

# Star Formation in Extreme Environments: The Effects of Cosmic Rays and Mechanical Heating.

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## ABSTRACT

**Context.** Molecular data of extreme environments, such as Arp 220, but also NGC 253, show evidence for extremely high cosmic ray (CR) rates ( $10^3 - 10^4 \times$  Milky Way) and mechanical heating from supernova driven turbulence.

**Aims.** The consequences of high CR rates and mechanical heating on the chemistry in clouds are explored.

**Methods.** PDR model predictions are made for low,  $n = 10^3$ , and high,  $n = 10^{5.5} \text{ cm}^{-3}$ , density clouds using well-tested chemistry and radiation transfer codes. Column densities of relevant species are discussed, and special attention is given to water related species. Fluxes are shown for fine-structure lines of O, C<sup>+</sup>, C, and N<sup>+</sup>, and molecular lines of CO, HCN, HNC, and HCO<sup>+</sup>. A comparison is made to an X-ray dominated region model.

**Results.** Fine-structure lines of [CII], [CI], and [OI] are remarkably similar for different mechanical heating and CR rates, when already exposed to large amounts of UV. HCN and H<sub>2</sub>O abundances are boosted for very high mechanical heating rates, while ionized species are relatively unaffected. OH<sup>+</sup> and H<sub>2</sub>O<sup>+</sup> are enhanced for very high CR rates  $\zeta \geq 5 \cdot 10^{-14} \text{ s}^{-1}$ . A combination of OH<sup>+</sup>, OH, H<sub>2</sub>O<sup>+</sup>, H<sub>2</sub>O, and H<sub>3</sub>O<sup>+</sup> trace the CR rates, and are able to distinguish between enhanced cosmic rays and X-rays.

**Key words.** Cosmic Rays – Mechanical Heating – Interstellar Medium – Excitation

## 1. Introduction

Observations of molecular tracers have suggested that both star formation and an active galactic nucleus (AGN, an accreting supermassive black hole) can drive the physics and chemistry of the central kpc of active galaxies (Sanders & Mirabel 1996; Gao et al. 1997; Gao & Solomon 1999; Baan et al. 2008; van der Werf et al. 2010). Specifically, Ultra-Luminous Infrared Galaxies (ULIRGs), with infrared (8 – 1000  $\mu\text{m}$ ) luminosities  $L_{\text{IR}} \geq 10^{12} L_{\odot}$ , appear to contain large reservoirs of dense,  $n > 10^4 \text{ cm}^{-3}$ , gas. This gas provides the fuel for (intense) star formation and black hole accretion.

The irradiation by UV photons (6–13.6 eV; creating so-called photon-dominated regions, or PDRs, e.g., Hollenbach & Tielens 1999) from a starburst or by X-rays (1–100 keV, creating so-called X-ray dominated regions, or XDRs, e.g., Lepp & Dalgarno 1996; Maloney et al. 1996) from an AGN is expected to produce different signatures in the molecular chemistry (Meijerink & Spaans 2005; Meijerink et al. 2006, 2007). Recently, mechanical heating due to supernova and stellar outflow driven turbulence has been explored as well (Loenen et al. 2008), which shows that warm molecular gas may persist beyond a few magnitudes of extinction in molecular clouds. Furthermore, the radiation feedback from ultraviolet photons, resulting in warm dust of more than 50 K, affect the thermodynamics of the molecular gas, possibly resulting in a top-heavy initial mass function (IMF; Klessen et al. 2007; Hocuk & Spaans 2010).

The analysis of the physical state of this irradiated gas allows one to constrain the evolutionary state of, ambient star formation rate in, and the importance of feedback for ULIRGs (Baan et al.

2010). In this work, we focus on feedback that results from massive stars. In particular, we consider UV emission from hot stars, the (elevated) production of cosmic rays from the resulting supernova remnants, and the heating that results from turbulent motions that are driven by travelling supernova blast waves.

A very nice case in point for the feedback effects mentioned above is Arp 220, the proto-typical ULIRG at 77 Mpc, which boasts a infrared luminosity of  $L_{\text{IR}} = 1.3 \cdot 10^{12} L_{\odot}$  (Soifer et al. 1987). Arp 220 is a merger and contains two nuclei separated by about 370 pc in the east-west direction (e.g., Rodríguez-Rico et al. 2005). The nuclear star formation rate of Arp 220 is  $50\text{--}100 M_{\odot} \text{ yr}^{-1}$  (Smith et al. 1998).

Observations of Arp 220 at a resolution of 0.3'' (100 pc) by Sakamoto et al. (2009) indicate P Cygni type profiles in HCO<sup>+</sup> 4-3, 3-2 and CO 3-2. These authors interpret their results as a  $\sim 100 \text{ km s}^{-1}$  outflow that is driven by supernova explosions (or radiation pressure from the starburst). Interestingly, as many as 49 supernova remnants (SNRs) have been detected with VLBI (1 pc resolution) at 18 cm by (Lonsdale et al. 2006), confirming the formation and demise of many massive stars. The latter authors derive a supernova rate of  $3 \text{ yr}^{-1}$  for the western nucleus and  $1 \text{ yr}^{-1}$  for the eastern nucleus, more than two orders of magnitude larger than the entire Milky Way.

Limits on the cosmic ray (CR) rate in our Milky Way are discussed by, e.g., Van der Tak & van Dishoeck (2000). They found a value of  $\zeta = 2.6 \pm 0.8 \cdot 10^{-17} \text{ s}^{-1}$  with upper limits that are 3 to 5 times higher. In this paper we adopt  $\zeta = 5 \cdot 10^{-17} \text{ s}^{-1}$  as the canonical Milky Way value. Highly elevated cosmic ray rates are seen in the recent Gamma ray observations of the starburst galaxy NGC 253 (Acero et al. 2009) with the High Energy

Stereoscopic System (H.E.S.S.) array. The observed gamma ray flux indicates a cosmic ray density that is three orders of magnitude larger than our Milky Way.

Papadopoulos (2010) suggests that ULIRGs generally have cosmic ray densities  $U_{\text{CR}} \sim 10^3 - 10^4 U_{\text{cr,MW}}$ , and discusses the impact on the ionization fraction and thermal state of the gas, and the consequences for the initial conditions for star-formation. In this paper, we first discuss the detailed effects of enhanced cosmic ray rates on both the thermal balance and chemistry (Section 2). Then, we will highlight the global consequences on the chemistry and suggest potential diagnostic species (Section 3), which is followed by the observational consequences (Section 4). In Section 5, we will conclude with the key diagnostics needed to derive quantitative and qualitative properties of interstellar medium (ISM) exposed to large amounts of cosmic rays, and show how it differs from gas exposed X-rays.

## 2. PDR models

We have constructed a set of PDR models (see Table 1) from the code as described by Meijerink & Spaans (2005) and Meijerink et al. (2007). We consider a low ( $n = 10^3 \text{ cm}^{-3}$ ), and a high density ( $n = 10^{5.5} \text{ cm}^{-3}$ ) phase. The low density phase of the ISM is generally not directly connected to starformation. Therefore, the adopted incident UV field in the low density models ( $G_0 = 10^3$ ) is chosen a factor 100 lower than the high density phase ( $G_0 = 10^5$ ) in order to reflect this and essentially corresponding to Model 1 and 4 in Meijerink & Spaans (2005). We varied the incident cosmic ray rates between  $\zeta = 5 \cdot 10^{-17} \text{ s}^{-1}$  and  $\zeta = 5 \cdot 10^{-13} \text{ s}^{-1}$ . The highest cosmic ray rate considered here is two orders of magnitude higher than in Meijerink et al. (2006). We adopt a Solar metallicity  $Z = Z_{\odot}$  and an abundance ratio  $[C]/[O] = 0.4$ , which is based on the average abundances of Asplund et al. (2005) and Jenkins (2004), and summarized in Table 2 of Meijerink & Spaans 2005.

We also consider the effect of mechanical heating in the high density case, specifically  $\Gamma_{\text{mech}} = 3.0 \cdot 10^{-18}$  and  $2.0 \cdot 10^{-17} \text{ erg cm}^{-3} \text{ s}^{-1}$ , which correspond to star formation rates of about  $SFR = 140$  and  $950 M_{\odot} \text{ yr}^{-1}$ , respectively, for a Salpeter IMF (see Loenen et al. 2008, for details). Mechanical heating is only considered in the high density case,  $n > 10^4 - 10^5 \text{ cm}^{-3}$ , since we expect this dense phase to be directly responsible for star formation and thus be affected directly by the supernovae from massive stars. We assume that the low density phase is only affected by cosmic rays. These are able to travel through large columns ( $N_{\text{H}} \sim 10^{24} \text{ cm}^{-2}$ ), since they have small absorption cross sections, and are likely to impact the ISM on larger scales.

The effects on the thermal balance and chemistry are discussed for Model sets 1a ( $G_0 = 10^5$ ;  $n = 10^{5.5} \text{ cm}^{-3}$ ), 1b and 1c (same as Model set 1a, with  $\Gamma_{\text{mech}} = 3.0 \cdot 10^{-18}$  and  $2.0 \cdot 10^{-17} \text{ erg cm}^{-3} \text{ s}^{-1}$ , respectively) and 2 ( $G_0 = 10^3$ ;  $n = 10^3 \text{ cm}^{-3}$ ) in order to highlight the differences between the high and low density phases of the ISM.

### 2.1. Thermal balance

The surface temperature for the high density model without boosting the CR rate (i.e.  $\zeta = 5 \cdot 10^{-17} \text{ s}^{-1}$ ) is higher than for the low density model. This may seem a little counterintuitive, since  $G_0/n=1$  (0.3) for the low (high) density model, and as a result there is more energy available per particle in the low density model. Besides that, cooling is more efficient at high

**Table 1.** Model parameters

Metallicity [ $Z_{\odot}$ ]	1.0		
[C]:[O] ratio	0.4		
CR rates [ $\text{s}^{-1}$ ]	$5 \cdot 10^{-17}, 5 \cdot 10^{-16}, 5 \cdot 10^{-15}, 5 \cdot 10^{-14}, 5 \cdot 10^{-13}$		
Model set	Density [ $\text{cm}^{-3}$ ]	Radiation field [ $G_0$ ]	$\Gamma_{\text{mech}}$ [ $\text{erg cm}^{-3} \text{ s}^{-1}$ ]
1a	$10^{5.5}$	$10^5$	0.0
1b	$10^{5.5}$	$10^5$	$3.0 \cdot 10^{-18}$
1c	$10^{5.5}$	$10^5$	$2.0 \cdot 10^{-17}$
2	$10^3$	$10^3$	0.0

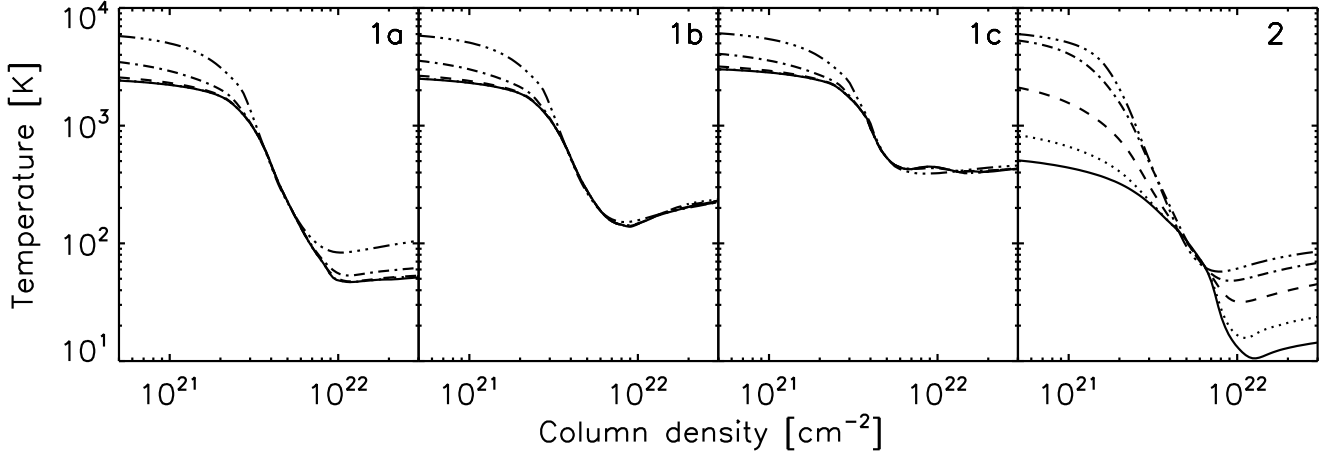
densities. However, at high radiation fields ( $G_0 > 10^4$ , and  $n > 10^4 - 10^5 \text{ cm}^{-3}$ ), the gas cooling thermalizes ( $\Lambda \propto n$  instead of  $n^2$ ), while photo-electric heating becomes more effective because of the higher electron density, and more effective than  $\Gamma \sim n$  (e.g., Kaufman et al. 1999; Meijerink et al. 2007).

The sensitivity of the thermal balance to cosmic rays is different for the high and low density phase (see Fig. 1). In Model set 1a, only very high CR rates ( $\zeta \geq 5 \cdot 10^{-14} \text{ s}^{-1}$ ) are able to increase the temperature significantly ( $\sim 25$  to 200 percent) in both the radical region (low  $A_V$ ) as well as the shielded molecular region. In Model sets 1b and 1c, mechanical heating in the shielded region of the cloud dominates over cosmic ray heating. Here, the temperatures overlap for all cosmic ray rates, reaching values  $T \sim 100 - 200 \text{ K}$  for Model set 1b and  $T \sim 400 \text{ K}$  for Model set 1c. So even for moderate mechanical heating rates (in this case corresponding to a  $SFR=140 M_{\odot}/\text{yr}$ ), the CR rate has no additional effect on the thermal balance in the shielded regions of clouds. In Model set 2, temperatures are increased for all CR rates at all column densities, up to an order of magnitude with the highest adopted CR rate. The effect on the thermal balance is larger, because cooling is simply less efficient at lower densities ( $\Lambda \propto n^2$ ), compared to the heating rate that is proportional to the density, ( $\Gamma \propto n$ ). This makes the low density models more sensitive to a larger heating rate. This is enhanced by the fact that the fractional electron abundance is increased more easily as well at lower densities ( $k_{\text{rec}} \propto n^2$ ), resulting in a higher heating efficiency (cf., Bakes & Tielens 1994), and higher heating rates.

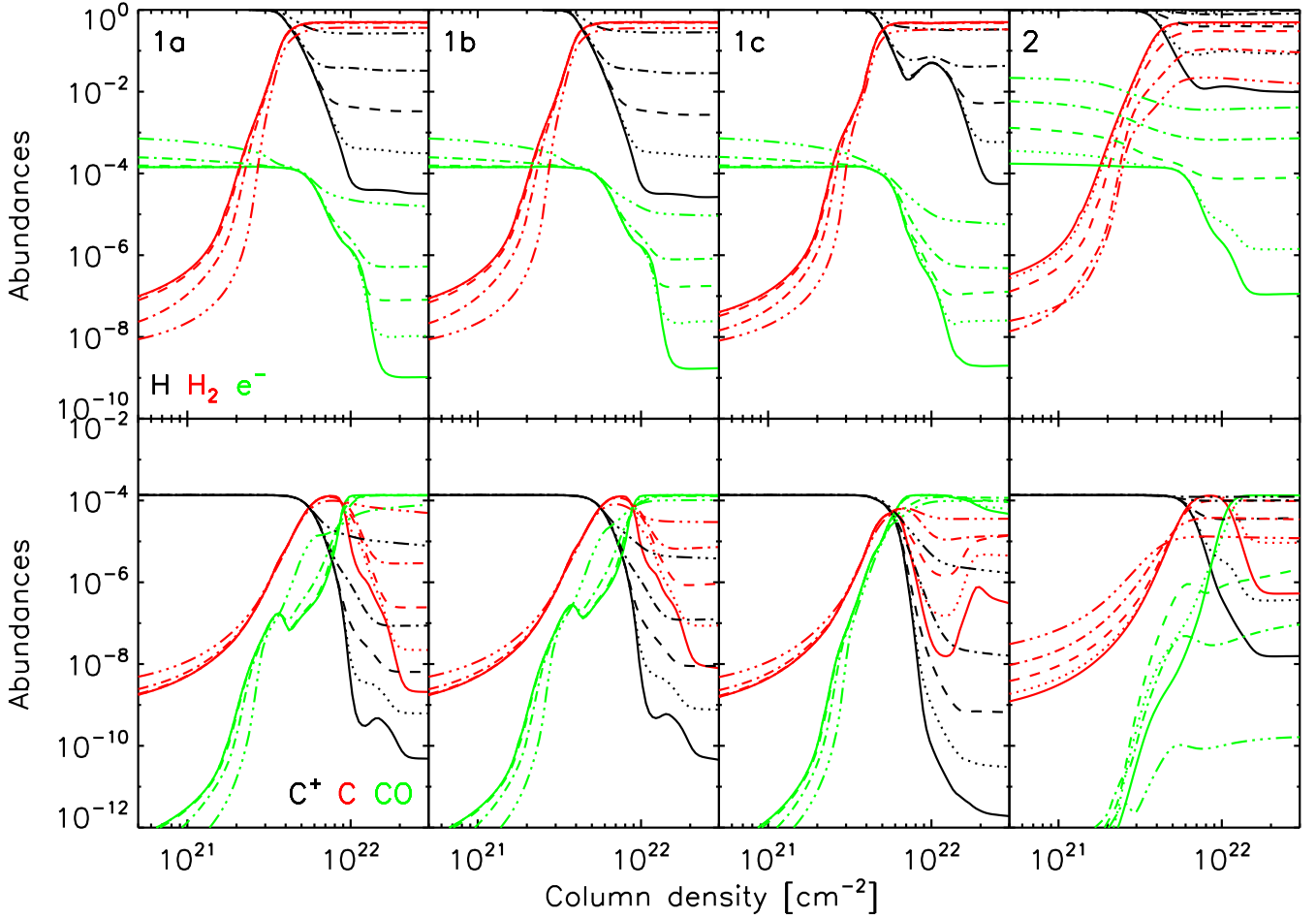
### 2.2. Chemical balance

**Electron abundances (Fig. 2):** The effect of cosmic rays is less apparent in the unshielded region ( $N_{\text{H}} \lesssim 3 \cdot 10^{21} \text{ cm}^{-2}$ ) than in the molecular region ( $N_{\text{H}} \gtrsim 10^{22} \text{ cm}^{-2}$ ) of the cloud, since charged species in the unattenuated part of cloud are also produced through photoionization by the stellar radiation field. Here, the fractional abundance (which is defined as  $x_i = n_i/n(\text{H} + 2\text{H}_2)$ ) of electrons varies between  $x_e \sim 10^{-4} - 10^{-3}$  ( $10^{-4} - 10^{-2}$ ) in the high (low) density models, while the CR rates vary over 4 orders of magnitude. In the molecular region, however, an order of magnitude higher CR rate gives a similar rise in the electron fractional abundance, giving ranges  $x_e \sim 10^{-9} - 10^{-5}$  and  $10^{-7} - 10^{-2}$  for the high and low density models, respectively. Adding mechanical heating (1b and 1c) does not change the electron abundance much. The difference in fractional electron abundance between the highest and lowest CR rate is somewhat larger than for the models without mechanical heating.

**H and H<sub>2</sub> abundances (Fig. 2):** Atomic hydrogen is by far the dominant species in the radical region ( $N_{\text{H}} \lesssim 2 - 3 \cdot 10^{22} \text{ cm}^{-2}$ ), but when the attenuating column becomes larger, molecular hydrogen becomes more and more abundant. For the



**Fig. 1.** Temperatures for all models sets (see Table 1) for cosmic ray rates  $\zeta = 5 \cdot 10^{-17}$  (solid line),  $5 \cdot 10^{-16}$  (dotted),  $5 \cdot 10^{-15}$  (dashed),  $5 \cdot 10^{-14}$  (dot-dashed), and  $5 \cdot 10^{-13} \text{ s}^{-1}$  (dotted-dashed).



**Fig. 2.** Abundances of H, H<sub>2</sub>, e<sup>-</sup>, C<sup>+</sup>, C and CO for all models sets (see Table 1). Line styles corresponding to the different CR rates are the same as in Fig. 1.

canonical CR rate ( $\zeta = 5 \cdot 10^{-17} \text{ s}^{-1}$ ), the atomic hydrogen abundance drops below  $x_{\text{H}} \sim 10^{-4}$  ( $10^{-2}$ ) for the high (low) density models. The H to H<sub>2</sub> transition becomes less and less complete for higher CR rates, which is due to CR reactions such as  $\text{H}_2 + \text{CR} \rightarrow \text{H} + \text{H}^+ + \text{e}^-$  and  $\text{H}_2 + \text{CR} \rightarrow \text{H}_2^+ + \text{e}^-$ . Atomic

and molecular hydrogen are of similar abundance for the highest adopted CR rate in the high density case, while atomic hydrogen is dominant for CR rates  $\zeta > 5 \cdot 10^{-15} \text{ s}^{-1}$  in the low density case.

**C<sup>+</sup>, C and CO abundances (Fig. 2):** Similar trends are seen for the C<sup>+</sup>/C/CO transition. For the lowest CR rate ( $\zeta =$

$5 \cdot 10^{-17} \text{ s}^{-1}$ ), there are three well defined zones where one species is most abundant. Increasing CR rates result in a larger neutral carbon abundance in the unattenuated part of the cloud by a factor of  $\sim 3$  ( $\sim 30$ ) in the high (low) density case. However, the abundances are still low compared to  $\text{C}^+$ . Again most effect is seen at large column density ( $N_{\text{H}} > 10^{22} \text{ cm}^{-2}$ ). The  $\text{C}^+$  and C abundances increase very fast with the CR rate. In the high density case, the  $\text{C}^+$  and C abundances become  $10^{-6} - 10^{-5}$  and  $3 - 6 \cdot 10^{-5}$ , respectively, depending on the amount of additional mechanical heating. There is no full transition to CO for  $\zeta \geq 10^{-15} \text{ s}^{-1}$  in the low density case. Neutral carbon is the dominant species at high column density  $\zeta = 5 \cdot 10^{-15} \text{ s}^{-1}$ , and  $\text{C}^+$  has become the dominant species at  $\zeta \geq 5 \cdot 10^{-14} \text{ s}^{-1}$ , and at the same time there is almost no CO left ( $x_{\text{CO}} < 10^{-6}$ ).

**$\text{H}^+$ ,  $\text{H}_2^+$ , and  $\text{H}_3^+$  abundances (Fig. 3):** The main drivers of chemistry in PDRs are ionic species, starting with species  $\text{H}^+$ ,  $\text{H}_2^+$ , and  $\text{H}_3^+$ .  $\text{H}^+$  and  $\text{H}_2^+$  are mainly (directly or indirectly) produced by cosmic ray ionization ( $\text{H} + \text{CR} \rightarrow \text{H}^+ + \text{e}^-$ ;  $\text{H}_2 + \text{CR} \rightarrow \text{H}_2^+ + \text{e}^-$  or  $\text{H}^+ + \text{H} + \text{e}^-$  or  $\text{H} + \text{H}$ ). UV photons of energy larger than 13.6 eV are all readily absorbed in a very small column, forming an HII region in front of the PDR.  $\text{H}_2$  can only be photodissociated to two hydrogen atoms (with an UV excited  $\text{H}_2^*$  as intermediate), no ionic species are produced by direct photoionization of  $\text{H}_2$ . Therefore, large effects on abundances of ionic species are seen by varying the cosmic ray rate.

In the unshielded region, the abundance increase of  $\text{H}^+$  and  $\text{H}_2^+$  scale with the ionization rate.  $\text{H}^+$  is directly produced by cosmic ray ionization. The  $\text{H}_2^+$  abundance is balanced by the charge exchange reactions  $\text{H}^+ + \text{H}_2 \leftrightarrow \text{H}_2^+ + \text{H}$ . The reaction to the right has an energy barrier of  $T \sim 20000 \text{ K}$ , and is only efficient at temperatures of a few thousand Kelvin. Therefore, the  $\text{H}_2^+$  abundance is still able to increase with CR rate: the smaller  $\text{H}_2$  abundance at higher CR rates is counteracted by a temperature increase (see Fig. 1). At slightly larger column densities ( $N_{\text{H}} \sim 3 \cdot 10^{21} \text{ cm}^{-2}$ ), the temperature drops and only  $\text{H}_2^+ + \text{H} \rightarrow \text{H}^+ + \text{H}_2$  is efficient, while simultaneously the H to  $\text{H}_2$  transition occurs. This together results in an abundance maximum of  $\text{H}^+$ , and also explains why the  $\text{H}_2^+$  abundance is not increasing as fast as the  $\text{H}_2$  abundance.

After the H to  $\text{H}_2$  transition ( $N_{\text{H}} \gtrsim 5 \cdot 10^{21} \text{ cm}^{-2}$ ), the overall ionization degree drops, which coincides with a decrease in temperature. This is mostly explained by recombination reactions (e.g.,  $\text{H}^+ + \text{e}^- \rightarrow \text{H} + \text{Photon}$ ), that are more efficient at lower temperatures. In this region, the increase of  $\text{H}^+$  with cosmic ray rate is faster than linear. The H to  $\text{H}_2$  transition is less complete for higher CR rates (Fig. 2), giving a larger reservoir of atomic hydrogen, that can potentially be ionized.

$\text{H}_3^+$  is formed and destroyed by  $\text{H}_2^+ + \text{H}_2 \rightarrow \text{H}_3^+ + \text{e}^-$  and  $\text{H}_3^+ + \text{e}^- \rightarrow 3\text{H}$  and  $\text{H}_2 + \text{H}$ , respectively. At low column densities, the  $\text{H}_3^+$  abundance is dropping with CR rates due to enhanced electron and reduced  $\text{H}_2$  abundances. At higher column densities,  $\text{H}_3^+$  increases for large CR rates, but not one to one with the CR rate, due to more efficient recombination and lower  $\text{H}_2$  abundances (especially in the low density models).

**$\text{CH}^+$ ,  $\text{CH}_2^+$ , and  $\text{CH}$  abundances (Fig. 3):** In the unshielded region of the cloud, the formation of  $\text{CH}^+$  occurs mainly through  $\text{C}^+ + \text{H}_2^* \rightarrow \text{CH}^+ + \text{H}$ , where  $\text{H}_2^*$  is vibrationally excited molecular hydrogen. Therefore, the  $\text{CH}^+$  abundances do not change much with cosmic ray rate in the unshielded region of the cloud. However, at larger column densities ( $N_{\text{H}} \sim 10^{22} \text{ cm}^{-2}$ ), the main route is through  $\text{H}_3^+ + \text{C}$ . At high density, both the  $\text{H}_3^+$  and C abundance increase orders of magnitude for the larger CR rates, and as a result the  $\text{CH}^+$  abundance as well, despite the increased electron abundance. In the low density case, the

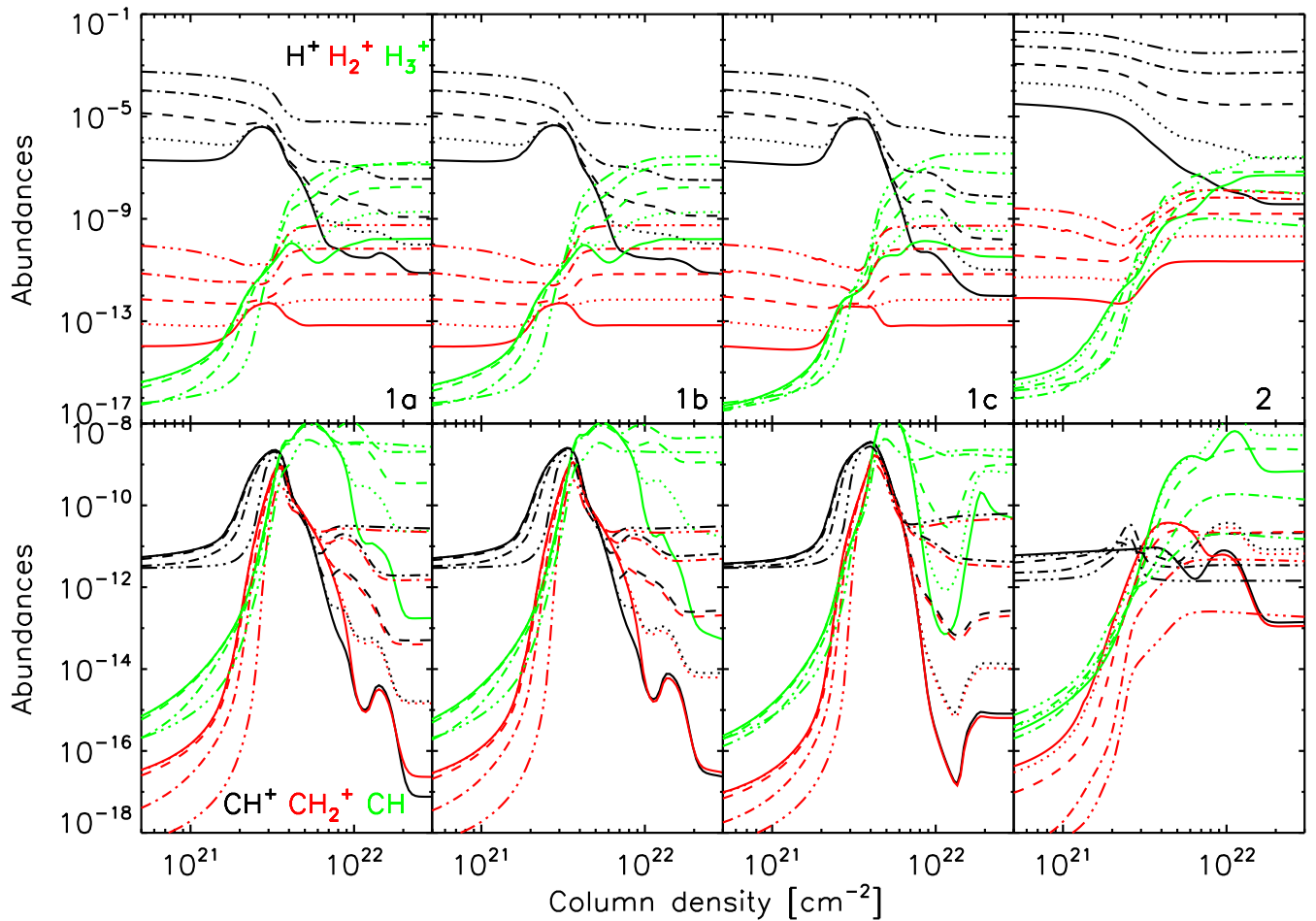
$\text{CH}^+$  abundances are very similar for all CR rates because there is no boost now through  $\text{C} + \text{H}_3^+$ .  $\text{CH}_2^+$  formation occurs mainly through  $\text{CH}^+ + \text{H}_2 \rightarrow \text{CH}_2^+ + \text{H}$  and follows the abundance of  $\text{CH}^+$  closely, except where molecular hydrogen is not the dominant species, i.e., the radical region in the high density case and for very high CR rates in the low density case.

CH can be formed by the neutral-neutral reactions  $\text{C} + \text{H}_2 \rightarrow \text{CH} + \text{H}$  and  $\text{C} + \text{OH} \rightarrow \text{CH} + \text{O}$ , which have energy barriers of  $T \sim 11700$  and  $14800 \text{ K}$ , respectively, and the recombination reaction  $\text{CH}_2^+ + \text{e}^- \rightarrow \text{CH} + \text{H}$ . Destruction happens through UV photodissociation and photoionization at small column densities, and by fast charge exchange reactions (e.g.,  $\text{H}^+ + \text{CH} \rightarrow \text{CH}^+ + \text{H}$ ) at all column densities. At small column densities ( $N_{\text{H}} \lesssim 10^{21} \text{ cm}^{-2}$ ), the CH abundances are fairly similar, and UV photoionization dominates the destruction, and neutral-neutral reactions formation. The small differences can be explained by small deviations in  $\text{H}_2$  and C abundances. At column densities  $N_{\text{H}} \gtrsim 5 \cdot 10^{21} \text{ cm}^{-2}$ , the formation is dominated by recombination of  $\text{CH}_2^+$ , and the abundance is mainly determined by the CR rate.

**Water chemistry (Fig. 4):**  $\text{H}_2\text{O}$  and related species,  $\text{OH}^+$ ,  $\text{OH}$ ,  $\text{H}_2\text{O}^+$ , and  $\text{H}_3\text{O}^+$  are significantly affected by cosmic rays. First we consider  $\text{H}_2\text{O}$ . It can be formed through the neutral-neutral reaction  $\text{H}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{H}$ , for which temperatures  $T > 200 - 300 \text{ K}$  are required. Cosmic rays are not able to increase the temperature to these temperatures, not even the highest cosmic ray rates. Another important route, especially when gas is significantly ionized by enhanced cosmic ray rates, is, e.g.,  $\text{H}_2^+ + \text{O} \rightarrow \text{OH}^+ + \text{H}$ , then  $\text{OH}^+ + \text{H}_2 \rightarrow \text{H}_2\text{O}^+ + \text{H}$ ,  $\text{H}_2\text{O}^+ + \text{H}_2 \rightarrow \text{H}_3\text{O}^+ + \text{H}$ , followed by recombination,  $\text{H}_3\text{O}^+ + \text{e}^- \rightarrow \text{H}_2\text{O} + \text{H}$ . Destruction is possible through UV photodissociation, charge exchange, proton transfer, ion-molecule reactions and cosmic rays. Important routes are  $\text{He}^+ + \text{H}_2\text{O} \rightarrow \text{OH} + \text{He} + \text{H}^+$  and  $\text{H}^+ + \text{H}_2\text{O} \rightarrow \text{H}_2\text{O}^+ + \text{H}$ , and varying the cosmic ray rates affect these abundances. Therefore, at intermediate column densities  $N_{\text{H}} \sim 3 \cdot 10^{21}$  to  $10^{22} \text{ cm}^{-2}$  in model sets 1a and 1b, the water abundances increase for higher CR rates. In these models, the temperatures are not high enough to form  $\text{H}_2\text{O}$  through neutral-neutral reactions. When the temperature is high enough to form water (model set 1c) through the neutral-neutral reactions, a higher ionization degree is a drawback ( $\text{H}_2\text{O}$  is destroyed by, e.g.,  $\text{He}^+$ ), and the water abundance decreases for very high CR rates ( $\zeta \gtrsim 5 \cdot 10^{-14} \text{ s}^{-1}$ ). In model set 2, there is not enough  $\text{H}_2$  at the higher cosmic ray rates to form water through ion-molecule reactions.

OH is formed through  $\text{H}_2 + \text{O} \rightarrow \text{OH} + \text{H}$  or destruction of water (see previous paragraph). In the radical region where temperatures are significant, formation through neutral reactions dominates. In the high density models they are closely connected to the  $\text{H}_2$  abundance, and here the OH abundance is slightly lower for the high CR rates. In the low density case, the OH abundance increases with CR rate in the radical region, since the temperature increases about an order of magnitude. When temperatures are lower, i.e.,  $N_{\text{H}} \gtrsim 5 \cdot 10^{21} \text{ cm}^{-2}$ , the contribution of water destruction becomes more important. OH abundances are significantly larger in model set 1a and 1b, when CR rates are higher. In model set 1c, formation through neutral-neutral reactions becomes more important, and the effect of an enhanced CR rate less evident.

$\text{OH}^+$  is formed by  $\text{H}^+ + \text{OH} \rightarrow \text{OH}^+ + \text{H}$  and  $\text{H}^+ + \text{O} \rightarrow \text{O}^+ + \text{H}$  followed by  $\text{O}^+ + \text{H}_2 \rightarrow \text{OH}^+ + \text{H}$  or by photoionization of OH. At small column densities, where  $\text{OH}^+$  abundances are very similar for different CR rates, the abundance is determined by the UV ionization of OH. At large column densities ( $N_{\text{H}} \gtrsim$



**Fig. 3.** Abundances of  $\text{H}^+$ ,  $\text{H}_2^+$ ,  $\text{H}_3^+$ ,  $\text{CH}$ ,  $\text{CH}^+$ , and  $\text{CH}_2^+$  for all model sets (see Table 1). Line styles corresponding to the different CR rates are the same as in Fig. 1.

$5 \cdot 10^{21} \text{ cm}^{-2}$ ), the UV is mostly gone, and here the  $\text{H}^+$  driven formation is more important, which is enhanced by cosmic rays.  $\text{H}_2\text{O}^+$  closely follows the  $\text{OH}^+$  abundance at these high column densities. It is mainly formed through  $\text{H}_2 + \text{OH}^+ \rightarrow \text{H}_2\text{O}^+ + \text{H}$ , and also very much enhanced at higher CR rates.

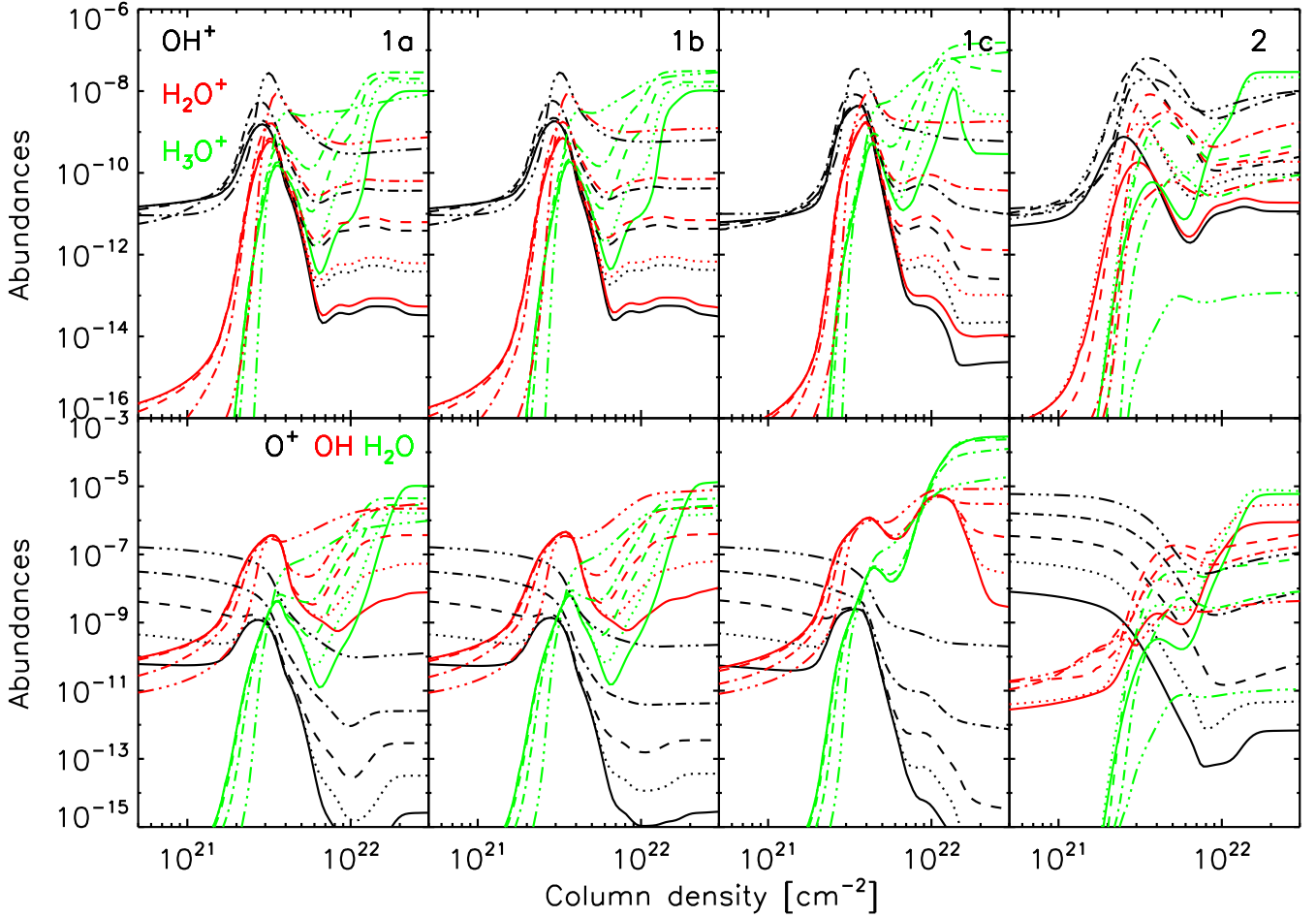
**Nitrogen chemistry (Fig. 5):**  $\text{N}^+$  has an ionization potential of 14.53 eV, which is too high for the available UV photons. This species shows orders of magnitude variations for all model sets. The species is strongly affected by the increased cosmic ray rate.  $\text{NH}^+$  and  $\text{NH}_2^+$  are closely connected to the cosmic ray rate at high column densities, because the formation is driven by  $\text{N} + \text{H}_2^+$  and  $\text{N}^+ + \text{H}_2$ .

$\text{HCN}$  and  $\text{HNC}$  do not show a strong response to enhanced CR rates in the high density case without mechanical heating, and the abundances remain similar for all CR rates. Adding mechanical heating (1b), however, drives the  $\text{HNC} + \text{H} \rightarrow \text{HCN} + \text{H}$  reaction that has a temperature barrier of  $T \sim 200 \text{ K}$ , and  $\text{HCN}$  has an abundance that is two orders of magnitude higher than  $\text{HNC}$ . In the low density case (2) both the  $\text{HCN}$  and  $\text{HNC}$  abundances, which are similar, decrease fast with increasing cosmic ray rates. This is a direct results of the decrease of  $\text{H}_2$  and  $\text{H}_3^+$ , which are important in the formation of these molecules.

**$\text{HCO}^+$  and CS (Fig. 6):** For Model sets 1a and 1b, the  $\text{HCO}^+$  abundances are enhanced with increasing CR rates. The formation occurs through  $\text{H}_3^+ + \text{CO} \rightarrow \text{HCO}^+ + \text{H}_2$ , which is fast at all temperatures, and is aided by  $\text{CH} + \text{O} \rightarrow \text{HCO}^+ + \text{e}^-$  at

high temperatures. Destruction happens through recombination with electrons but also through reactions with molecules such as  $\text{H}_2\text{O}$ ,  $\text{OH}$ , and  $\text{HCN}$ . In Model set 1b, the abundances of these species are especially enhanced for the lower ( $\zeta = 5 \cdot 10^{-17}$  and  $5 \cdot 10^{-16} \text{ s}^{-1}$ ) cosmic ray rates as discussed in the previous paragraphs, and suppress the  $\text{HCO}^+$  abundance compared to the models without mechanical heating. In the low density models (2), where the full transition to  $\text{H}_2$  does not occur, the  $\text{H}_3^+$  abundance is automatically suppressed as well, giving smaller abundances with increasing cosmic ray rates.

The sulfur chemistry contains many reactions with activation barriers.  $\text{CS}$  has two formation channels, the first through  $\text{S} + \text{CH} \rightarrow \text{CS} + \text{H}$  and the second through  $\text{S} + \text{H}_2 \rightarrow \text{HS} + \text{H}$  (with an energy barrier of  $T \sim 6000 \text{ K}$ ) followed by  $\text{HS} + \text{C} \rightarrow \text{CS} + \text{H}$ .  $\text{CS}$  is most abundant at column densities  $N_{\text{H}} \gtrsim 5 \cdot 10^{21} \text{ cm}^{-2}$ , where temperatures are not such that the second channel is very effective, although not insignificant in Model set 2. The formation of  $\text{CH}$  on the other hand is dependent on  $\text{H}_3^+$ , of which the abundance is highly dependent on CR rate. Destruction happens through ion-molecule reactions with, e.g.,  $\text{He}^+$ ,  $\text{H}^+$ ,  $\text{H}_3^+$ , that are also dependent on CR rate. The abundance is a very complex interplay between temperature and ionization rates (cf., Leen & Graff 1988; Meijerink et al. 2008). The abundance of  $\text{CS}$  increases with CR rate in Model set 1a and 1b, while Model set 1c shows a drop. Molecule formation becomes more and more ineffective in the low density case, and the  $\text{CS}$  abundance de-



**Fig. 4.** Abundances of  $\text{OH}^+$ ,  $\text{H}_2\text{O}^+$ ,  $\text{H}_3\text{O}^+$ ,  $\text{O}^+$ ,  $\text{OH}$ , and  $\text{H}_2\text{O}$  for all models sets (see Table 1). Line styles corresponding to the different CR rates are the same as in Fig. 1.

creases significantly with CR rates, similar to, e.g., HCN and HNC.

### 3. Integrated column densities

#### 3.1. Trends

The integrated column densities for the total cloud ( $N_{\text{H}} = 3 \cdot 10^{22} \text{ cm}^{-2}$ ) are shown in Tables 2 through 5 for the species discussed in the previous section. The main results are summarized in Fig. 7.

**Hydrogen chemistry (top row Fig. 7):** The integrated column densities of atomic and molecular hydrogen vary over a factor of 3 (10) for the high (low) density models over the whole range of cosmic ray rates. The ionic species of hydrogen,  $\text{H}^+$ ,  $\text{H}_2^+$ , and  $\text{H}_3^+$  show much larger variations. The column densities of  $N(\text{H}^+)$  vary from  $\sim 10^{16} - 10^{18} \text{ cm}^{-2}$  ( $10^{17} - 10^{20} \text{ cm}^{-2}$ ) for the high (low density models).  $\text{H}_3^+$  increases (decreases) 4 (2) orders of magnitude in the high (low) density case.

**Water chemistry (row 2 and 3 of Fig. 7):** The  $\text{O}^+$  column densities show a nice correlation with CR rate, and increases 2 to 3 orders of magnitude over the range of considered CR rates. Although there are large variations in absolute column densities for OH and  $\text{H}_2\text{O}$  between the different models, the OH/ $\text{H}_2\text{O}$  ratio increases with cosmic ray rate, from  $N(\text{OH})/N(\text{H}_2\text{O}) \sim 4 \cdot 10^{-3}$  ( $\sim 0.2$ ) to  $\sim 1 - 3$  ( $\sim 400$ ) for the high (low) density models.

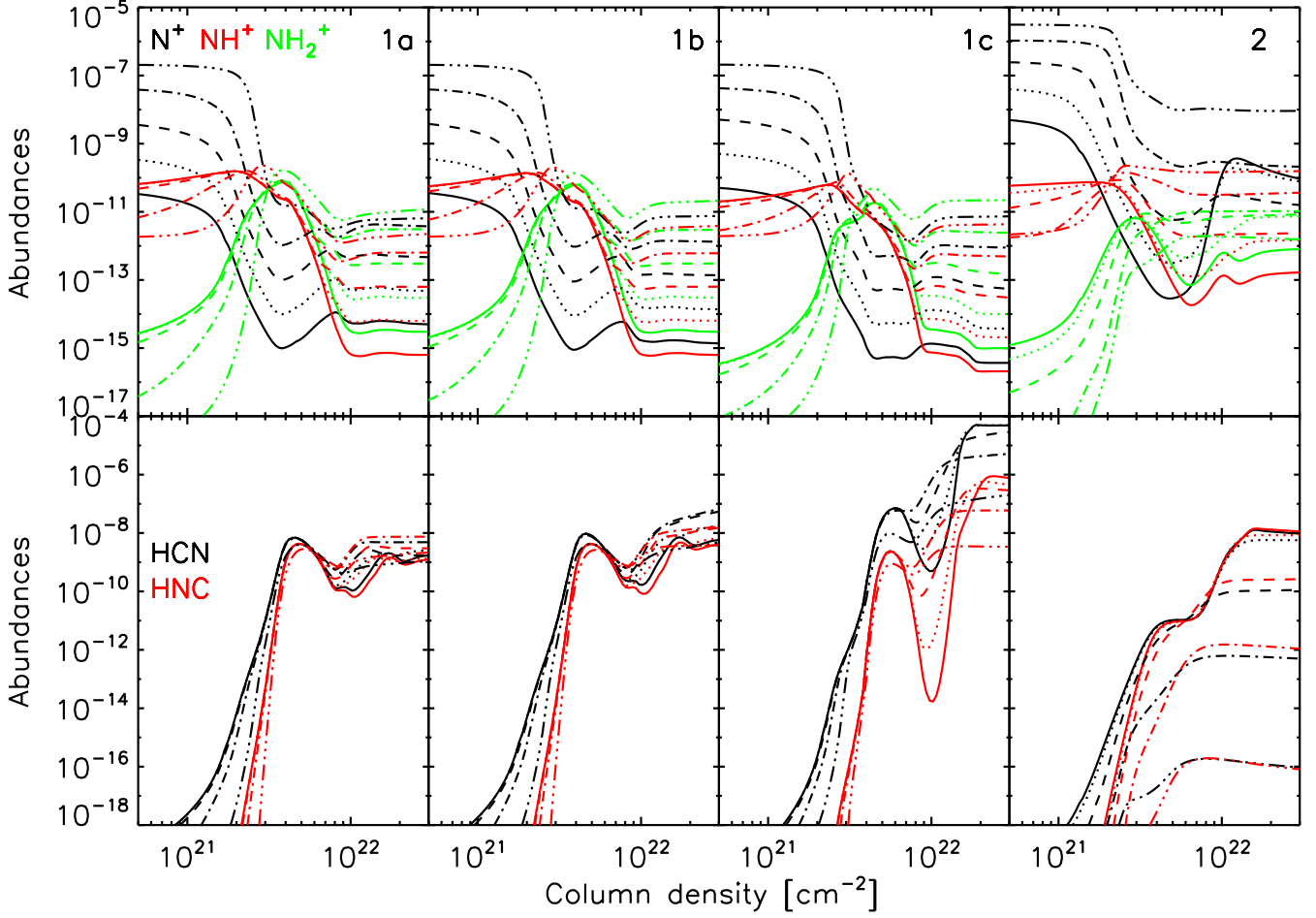
The  $\text{OH}^+$  and  $\text{H}_2\text{O}^+$  show a strong response to the CR rate for  $\zeta \gtrsim 5 \cdot 10^{-15} \text{ s}^{-1}$  in the high density case. Above this threshold, the column density increases with a factor  $\sim 10 - 20$  for  $\text{OH}^+$  and  $\sim 50 - 60$  for  $\text{H}_2\text{O}^+$ . In the low density case, the column densities for both species show a steep rise with CR rate up to  $\zeta \sim 5 \cdot 10^{-14} \text{ s}^{-1}$ , after which it levels off for  $\text{OH}^+$  and decreases for  $\text{H}_2\text{O}^+$ . The trends of  $\text{H}_3\text{O}^+$  generally show an increase (decrease) with CR rate in the high (low) density case. The response is more direct when high mechanical heating is added and temperatures are higher.

**$\text{CO}^+$  and  $\text{HCO}^+$  (row 4 in Fig. 7):**  $\text{HCO}^+$  does not show an obvious trend with increasing CR rates in the high density case. The  $\text{HCO}^+$  abundance anti-correlates with CR rate in the low density case. It does not seem to be a tracer that can be easily used as a CR tracer, but it does provide information when used in combination with e.g. the water chemistry.  $\text{CO}^+$  is very irresponsive to the CR rates at high density except for very high CR rates ( $\zeta > 5 \cdot 10^{-14} \text{ s}^{-1}$ ). In the low density case,  $N(\text{CO}^+)$  does not show a very obvious trend.

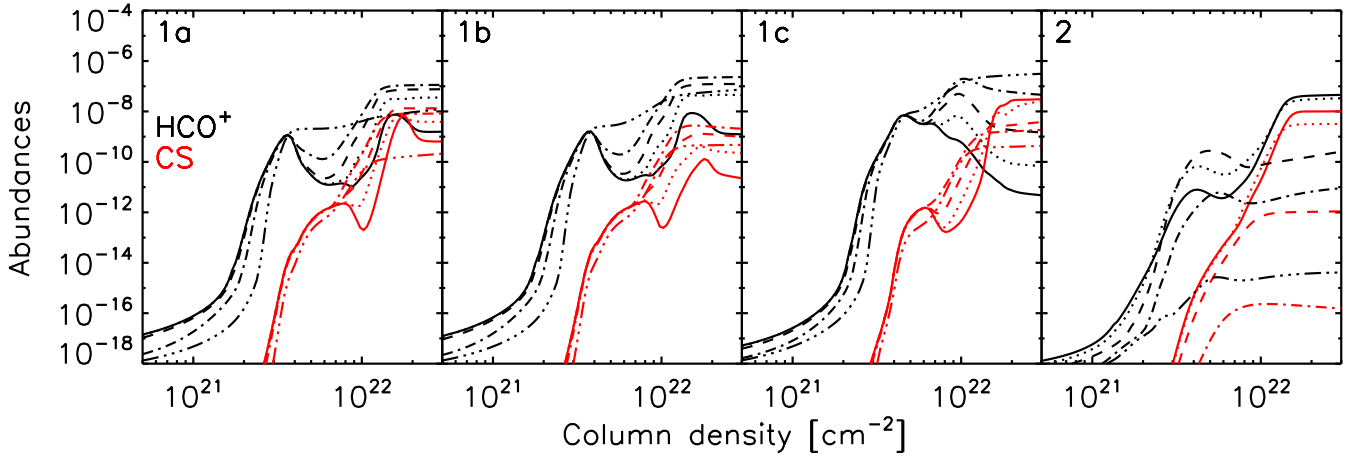
**$\text{C}^+$ ,  $\text{N}^+$ , and  $\text{C}$  (bottom row in Fig. 7):** Neutral and singly ionized carbon have very constant column densities over the range of CR rates considered.  $\text{N}^+$  on the other hand correlates very well with the CR rates, and therefore the  $\text{N}^+/\text{C}$  or  $\text{N}^+/\text{C}^+$  column density ratio can be diagnostic in estimating the CR rate.

**Other species:** Despite the fact that many species show large local variations in a cloud when varying CR rates, it does not al-





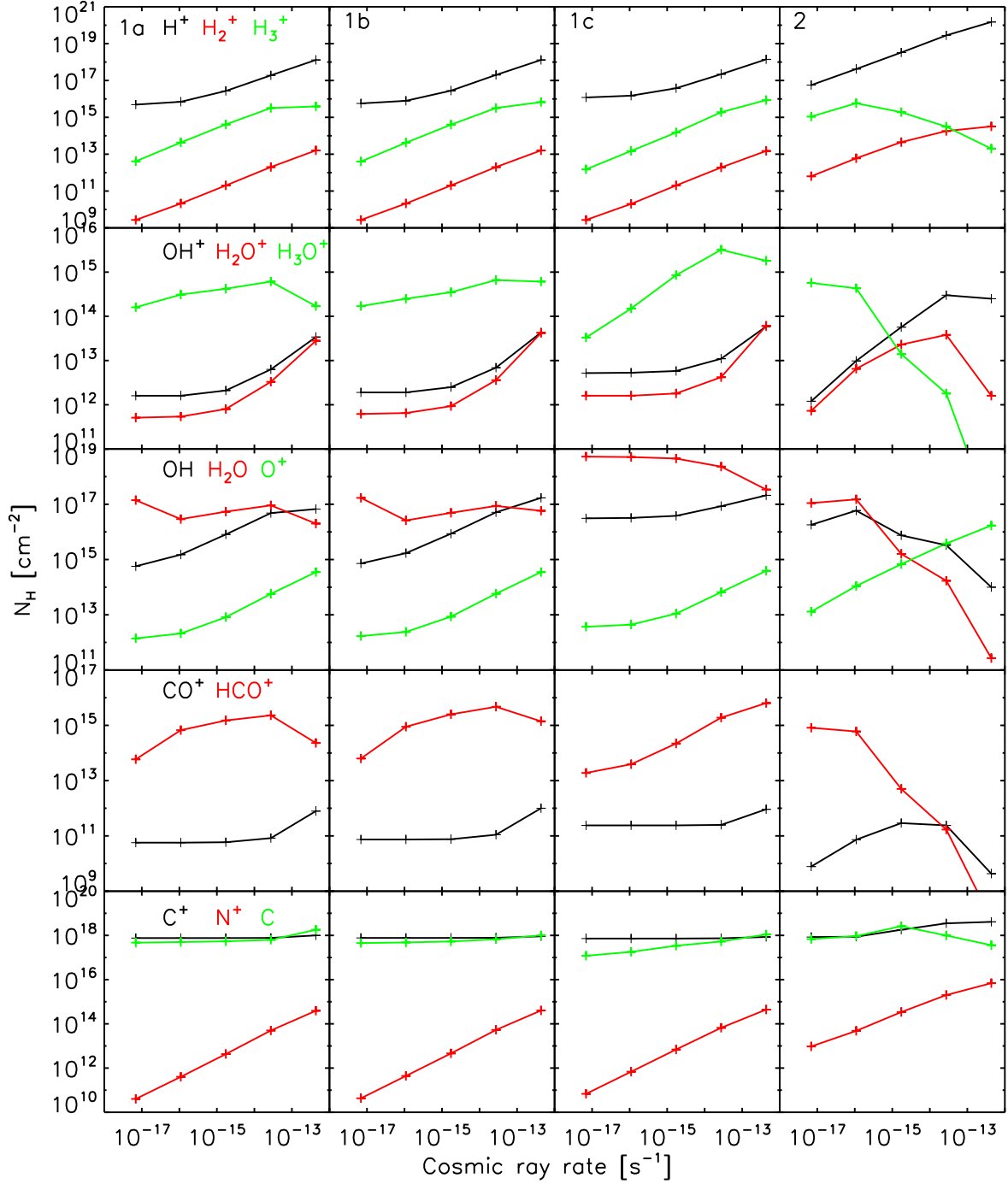
**Fig. 5.** Abundances of  $N^+$ ,  $NH^+$ ,  $NH_2^+$ ,  $HCN$ , and  $HNC$  for all models sets (see Table 1). Line styles corresponding to the different CR rates are the same as in Fig. 1.



**Fig. 6.** Abundances of  $HCO^+$  and  $CS$  for all model sets (see Table 1). Line styles corresponding to the different CR rates are the same as in Fig. 1.

ways result in significant changes in the integrated column densities in high density clouds. Examples are  $CH^+$  and  $CH_2^+$  which are the same within 5 percent over the whole range. In the low density models, variations are larger, but the integrated column densities are 1 or 2 orders of magnitude smaller. There are also

species that are not easy to interpret, such as  $NH^+$  and  $NH_2^+$ . The trends show a minimum or a maximum, when varying the CR rates. A number of species we considered have a strong dependence on temperature and ionization rate. Especially  $CS$  exhibits a very complex interplay, and does not show a particular trend.



**Fig. 7.** Column densities of diagnostic species.

### 3.2. Uncertainties

Molecular hydrogen,  $H_2$ , is a key species in the chemistry of the ISM. The formation of  $H_2$ , which mainly occurs on grain surfaces at these densities and metallicity, depend on the specific properties and temperatures of the grains, and is subject to a considerable uncertainty (cf., Cazaux & Tielens 2004). As a result the  $H_2$  abundance is uncertain as well, especially when the gas is not predominantly molecular, i.e., in the radical region.

Therefore, the column densities of key species such as  $O^+$ ,  $OH$ ,  $OH^+$ , and  $H_2O^+$  might be affected, especially when the in-

tegrated column density is dominated by the abundances in the radical region. In order to investigate this, we lowered the  $H_2$  formation rate by a factor 3, and here we summarize the results for some of the species, considering Model set 1a:

**$H_2$ ,  $H_2^+$ , and  $H^+$ :** The abundance of  $H_2$  is lower by a factor of  $\sim 3$  in the unshielded region of the cloud, and the  $H$  to  $H_2$  transition occurs now more gradual. In the molecular region, there is only a noticeable effect when there is no full transition to  $H_2$ , which is for the highest considered CR rate,  $\zeta = 5 \cdot 10^{-13} \text{ s}^{-1}$ . The column density of atomic hydrogen is  $\sim 10$  percent higher for the lowest up to  $\sim 80$  percent higher for the highest CR rate.



**Table 2.** Column densities for Model set 1a

Species	Cosmic ray rate ( $\text{s}^{-1}$ )				
	5(-17)	5(-16)	5(-15)	5(-14)	5(-13)
Column densities ( $\text{cm}^{-2}$ )					
H	4.2(21)	4.2(21)	4.3(21)	5.2(21)	1.2(22)
H <sub>2</sub>	1.4(22)	1.4(22)	1.4(22)	1.4(22)	1.0(22)
H <sup>+</sup>	4.9(15)	7.0(15)	2.7(16)	1.9(17)	1.3(18)
H <sub>2</sub> <sup>+</sup>	2.7(09)	2.1(10)	2.0(11)	2.0(12)	1.6(13)
H <sub>3</sub> <sup>+</sup>	4.1(12)	4.3(13)	4.1(14)	3.2(15)	3.9(15)
e <sup>-</sup>	8.1(17)	8.1(17)	8.4(17)	1.0(18)	2.5(18)
CH <sup>+</sup>	2.8(12)	2.7(12)	2.7(12)	2.4(12)	2.0(12)
CH <sub>2</sub> <sup>+</sup>	8.7(11)	8.7(11)	8.7(11)	8.4(11)	9.4(11)
CH	3.1(13)	3.3(13)	5.2(13)	1.1(14)	8.7(13)
O	6.6(18)	6.4(18)	6.4(18)	6.8(18)	9.3(18)
O <sup>+</sup>	1.4(12)	2.1(12)	8.2(12)	5.7(13)	3.5(14)
OH <sup>+</sup>	1.6(12)	1.6(12)	2.1(12)	6.3(12)	3.4(13)
H <sub>2</sub> O <sup>+</sup>	5.1(11)	5.4(11)	8.0(11)	3.3(12)	2.8(13)
H <sub>3</sub> O <sup>+</sup>	1.6(14)	3.1(14)	4.2(14)	6.1(14)	1.7(14)
OH	5.7(14)	1.5(15)	8.1(15)	4.8(16)	6.7(16)
H <sub>2</sub> O	1.4(17)	2.9(16)	5.4(16)	9.1(16)	2.0(16)
C <sup>+</sup>	7.6(17)	7.6(17)	7.6(17)	7.7(17)	1.0(18)
C	4.7(17)	5.0(17)	5.4(17)	6.3(17)	1.8(18)
CO	3.2(18)	3.2(18)	3.2(18)	3.1(18)	1.7(18)
CO <sup>+</sup>	5.7(10)	5.7(10)	5.9(10)	8.3(10)	7.9(11)
HCO <sup>+</sup>	5.9(13)	6.7(14)	1.5(15)	2.3(15)	2.3(14)
N <sup>+</sup>	4.0(10)	4.0(11)	4.3(12)	5.0(13)	3.9(14)
NH <sup>+</sup>	3.5(11)	3.5(11)	3.3(11)	2.9(11)	3.9(11)
NH <sub>2</sub> <sup>+</sup>	1.3(11)	1.3(11)	1.4(11)	2.3(11)	5.7(11)
HCN	4.3(13)	5.7(13)	5.6(13)	1.2(14)	3.2(13)
HNC	2.9(13)	3.5(13)	7.6(13)	1.8(14)	5.0(13)
CS	3.1(13)	8.4(13)	2.5(14)	1.6(14)	3.9(12)

Note - Numbers in parentheses:  $a(b) = a \cdot 10^b$ .**Table 3.** Column densities for Model set 1b

Species	Cosmic ray rate ( $\text{s}^{-1}$ )				
	5(-17)	5(-16)	5(-15)	5(-14)	5(-13)
Column densities ( $\text{cm}^{-2}$ )					
H	4.2(21)	4.3(21)	4.3(21)	5.1(21)	1.3(22)
H <sub>2</sub>	1.4(22)	1.4(22)	1.4(22)	1.4(22)	1.0(22)
H <sup>+</sup>	5.7(15)	7.9(15)	2.8(16)	2.0(17)	1.3(18)
H <sub>2</sub> <sup>+</sup>	2.7(09)	2.1(10)	2.0(11)	2.0(12)	1.6(13)
H <sub>3</sub> <sup>+</sup>	4.0(12)	4.2(13)	4.0(14)	3.2(15)	6.7(15)
e <sup>-</sup>	8.2(17)	8.2(17)	8.5(17)	1.0(18)	2.3(18)
CH <sup>+</sup>	3.2(12)	3.2(12)	3.1(12)	2.9(12)	2.3(12)
CH <sub>2</sub> <sup>+</sup>	1.0(12)	1.0(12)	1.0(12)	1.0(12)	9.8(11)
CH	3.1(13)	3.3(13)	7.0(13)	1.6(14)	5.9(13)
O	6.6(18)	6.6(18)	6.7(18)	7.0(18)	8.1(18)
O <sup>+</sup>	1.7(12)	2.4(12)	8.6(12)	5.8(13)	3.5(14)
OH <sup>+</sup>	1.9(12)	1.9(12)	2.5(12)	6.9(12)	4.3(13)
H <sub>2</sub> O <sup>+</sup>	6.2(11)	6.5(11)	9.3(11)	3.6(12)	4.2(13)
H <sub>3</sub> O <sup>+</sup>	1.7(14)	2.5(14)	3.5(14)	6.6(14)	6.1(14)
OH	7.2(14)	1.7(15)	8.6(15)	5.1(16)	1.7(17)
H <sub>2</sub> O	1.7(17)	2.6(16)	4.9(16)	8.7(16)	5.8(16)
C <sup>+</sup>	7.7(17)	7.7(17)	7.7(17)	7.8(17)	9.1(17)
C	4.5(17)	4.8(17)	5.3(17)	6.7(17)	1.0(18)
CO	3.2(18)	3.2(18)	3.2(18)	3.0(18)	2.5(18)
CO <sup>+</sup>	7.4(10)	7.4(10)	7.6(10)	1.1(11)	1.0(12)
HCO <sup>+</sup>	6.3(13)	8.9(14)	2.5(15)	4.7(15)	1.4(15)
N <sup>+</sup>	4.3(10)	4.4(11)	4.6(12)	5.3(13)	4.0(14)
NH <sup>+</sup>	3.1(11)	3.1(11)	2.9(11)	2.5(11)	3.8(11)
NH <sub>2</sub> <sup>+</sup>	1.1(11)	1.1(11)	1.2(11)	2.0(11)	7.3(11)
HCN	1.2(14)	2.8(14)	8.0(14)	9.5(14)	9.0(13)
HNC	7.5(13)	1.1(14)	2.5(14)	3.1(14)	8.9(13)
CS	8.6(11)	5.2(12)	2.3(13)	5.0(13)	1.0(13)

**Table 4.** Column densities for Model set 1c

Species	Cosmic ray rate ( $\text{s}^{-1}$ )				
	5(-17)	5(-16)	5(-15)	5(-14)	5(-13)
Column densities ( $\text{cm}^{-2}$ )					
H	5.1(21)	5.1(21)	5.3(21)	6.2(21)	1.4(22)
H <sub>2</sub>	1.4(22)	1.4(22)	1.4(22)	1.3(22)	9.3(21)
H <sup>+</sup>	1.2(16)	1.5(16)	3.8(16)	2.2(17)	1.4(18)
H <sub>2</sub> <sup>+</sup>	2.7(09)	2.0(10)	2.0(11)	1.9(12)	1.5(13)
H <sub>3</sub> <sup>+</sup>	1.5(12)	1.5(13)	1.5(14)	1.9(15)	8.6(15)
e <sup>-</sup>	7.8(17)	7.8(17)	8.1(17)	1.0(18)	2.3(18)
CH <sup>+</sup>	5.7(12)	5.7(12)	5.6(12)	5.5(12)	5.2(12)
CH <sub>2</sub> <sup>+</sup>	1.9(12)	1.9(12)	1.9(12)	1.9(12)	2.1(12)
CH	2.9(13)	3.8(13)	4.5(13)	7.4(13)	6.2(13)
O	3.2(18)	3.2(18)	3.4(18)	5.1(18)	7.8(18)
O <sup>+</sup>	3.7(12)	4.4(12)	1.1(13)	6.6(13)	3.9(14)
OH <sup>+</sup>	5.2(12)	5.3(12)	5.8(12)	1.1(13)	5.9(13)
H <sub>2</sub> O <sup>+</sup>	1.6(12)	1.6(12)	1.8(12)	4.2(12)	6.1(13)
H <sub>3</sub> O <sup>+</sup>	3.3(13)	1.5(14)	8.5(14)	3.2(15)	1.8(15)
OH	3.1(16)	3.2(16)	3.8(16)	8.5(16)	2.1(17)
H <sub>2</sub> O	5.3(18)	5.1(18)	4.5(18)	2.3(18)	3.4(17)
C <sup>+</sup>	7.2(17)	7.2(17)	7.2(17)	7.4(17)	8.5(17)
C	1.2(17)	1.8(17)	3.4(17)	5.3(17)	1.1(18)
CO	2.3(18)	2.5(18)	2.9(18)	3.1(18)	2.5(18)
CO <sup>+</sup>	2.4(11)	2.4(11)	2.4(11)	2.5(11)	9.2(11)
HCO <sup>+</sup>	1.9(13)	3.9(13)	2.2(14)	1.9(15)	6.4(15)
N <sup>+</sup>	6.8(10)	6.8(11)	6.9(12)	6.6(13)	4.4(14)
NH <sup>+</sup>	1.4(11)	1.3(11)	1.3(11)	1.2(11)	2.7(11)
NH <sub>2</sub> <sup>+</sup>	3.5(10)	3.5(10)	4.1(10)	1.0(11)	6.1(11)
HCN	8.0(17)	8.2(17)	4.4(17)	9.5(16)	3.5(15)
HNC	1.1(16)	8.0(15)	5.5(15)	1.2(15)	8.0(13)
CS	4.6(14)	3.2(14)	6.3(13)	3.5(13)	8.9(12)

Molecular hydrogen column densities only change significantly for the highest two CR rates,  $\sim 20$  and  $\sim 40$  percent lower, respectively.

The H<sup>+</sup> column density is lower by a factor  $\sim 3$  for the lowest and  $\sim 5$  to  $\sim 15$  percent higher for the highest two CR rates. The H<sup>+</sup> column density is dominated by  $\text{H}_2^+ + \text{H} \rightarrow \text{H}^+ + \text{H}_2$  in the radical region at  $\zeta = 5 \cdot 10^{-17} \text{ s}^{-1}$  and thus lower, while at higher CR rates the column density is increased because of the only partial transition to H<sub>2</sub>.

**O<sup>+</sup>, OH, OH<sup>+</sup>, H<sub>2</sub>O and H<sub>2</sub>O<sup>+</sup>, and H<sub>3</sub>O<sup>+</sup>:** The trend seen for the O<sup>+</sup> column density is very close to what is seen for H<sup>+</sup>, i.e., a factor of  $\sim 3$  lower for  $\zeta = 5 \cdot 10^{-17} \text{ s}^{-1}$ , while slightly higher for the highest CR rates. Similar trends are seen for OH<sup>+</sup> and H<sub>2</sub>O<sup>+</sup>.

H<sub>2</sub>O is only significantly affected (lowered by a factor  $\sim 2$ ) at the highest CR rate. OH column density is lower by a factor  $\sim 3$  for the lowest CR rates, and dominated by the abundance in the unshielded region of the cloud. This difference is much less (5-30 percent) for the higher CR rates. H<sub>2</sub>O and H<sub>3</sub>O<sup>+</sup> column densities are only affected for the highest two CR rates.

In all we conclude that the overall trends are not affected by uncertainties in the H<sub>2</sub> abundance, the main driver of the species of interest in our paper. The largest changes are seen when the integrated column density of a species is dominated by its abundance in the radical region, i.e., in the models with small CR rates.

**Table 5.** Column densities for Model set 2

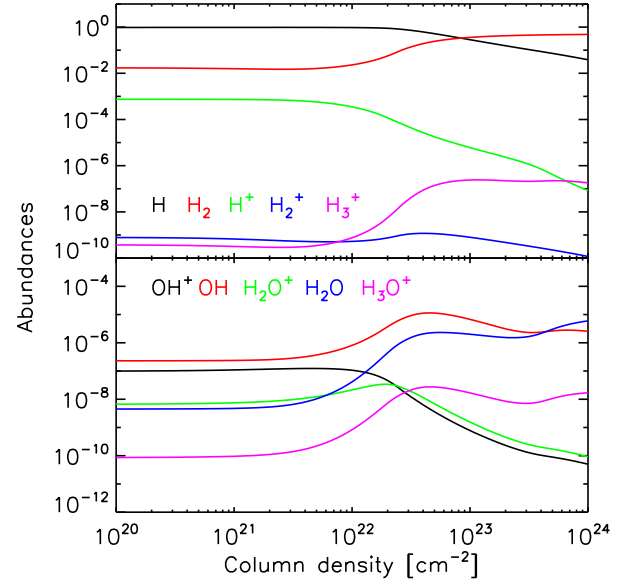
Species	Cosmic ray rate ( $s^{-1}$ )				
	5(-17)	5(-16)	5(-15)	5(-14)	5(-13)
Column densities ( $cm^{-2}$ )					
H	4.4(21)	6.6(21)	1.6(22)	2.7(22)	3.2(22)
H <sub>2</sub>	1.4(22)	1.3(22)	8.6(21)	2.8(21)	5.2(20)
H <sup>+</sup>	5.6(16)	4.2(17)	3.3(18)	2.8(19)	1.5(20)
H <sub>2</sub> <sup>+</sup>	6.3(11)	6.0(12)	4.5(13)	1.8(14)	3.2(14)
H <sub>3</sub> <sup>+</sup>	1.1(15)	5.8(15)	1.9(15)	3.1(14)	2.0(13)
e <sup>-</sup>	9.5(17)	1.4(18)	5.5(18)	3.4(19)	1.7(20)
CH <sup>+</sup>	7.9(10)	4.1(11)	5.8(11)	1.3(11)	5.7(10)
CH <sub>2</sub> <sup>+</sup>	1.4(11)	3.9(11)	6.5(11)	1.3(11)	6.1(09)
CH	4.5(13)	1.7(14)	6.0(13)	4.3(12)	4.7(11)
O	6.8(18)	7.8(18)	1.1(19)	1.1(19)	1.1(19)
O <sup>+</sup>	1.3(13)	1.1(14)	6.8(14)	3.8(15)	1.7(16)
OH <sup>+</sup>	1.2(12)	9.8(12)	5.7(13)	3.0(14)	2.5(14)
H <sub>2</sub> O <sup>+</sup>	7.3(11)	6.5(12)	2.3(13)	3.8(13)	1.6(12)
H <sub>3</sub> O <sup>+</sup>	5.7(14)	4.3(14)	1.4(13)	1.8(12)	3.0(09)
OH	1.8(16)	5.9(16)	7.5(15)	3.3(15)	1.0(14)
H <sub>2</sub> O	1.1(17)	1.5(17)	1.6(15)	1.7(14)	2.7(11)
C <sup>+</sup>	8.4(17)	8.7(17)	1.8(18)	3.5(18)	4.1(18)
C	6.8(17)	9.3(17)	2.6(18)	9.9(17)	3.6(17)
CO	2.9(18)	2.7(18)	4.0(16)	1.8(15)	3.9(12)
CO <sup>+</sup>	7.8(09)	7.3(10)	2.9(11)	2.4(11)	4.3(09)
HCO <sup>+</sup>	8.2(14)	6.0(14)	5.0(12)	1.7(11)	9.7(07)
N <sup>+</sup>	9.5(12)	4.8(13)	3.4(14)	2.0(15)	6.9(15)
NH <sup>+</sup>	1.8(11)	1.8(11)	2.2(11)	1.3(12)	4.8(12)
NH <sub>2</sub> <sup>+</sup>	2.6(10)	1.6(11)	2.3(11)	3.0(11)	4.9(10)
HCN	2.2(14)	1.2(14)	2.6(12)	1.5(10)	3.5(06)
HNC	2.5(14)	1.8(14)	6.1(12)	3.4(10)	3.3(06)
CS	1.8(14)	6.2(13)	2.5(10)	4.9(06)	3.2(03)

#### 4. Integrated line fluxes

Line fluxes for a number of species discussed in the previous section are shown in Tables 6 through 9. Here we highlight the main results:

**Fine-structure lines:** The two important cooling lines, [OI] 63  $\mu m$  and [CII] 158  $\mu m$ , that mainly determine the energy budget of interstellar clouds, have very similar fluxes for different CR rates in the high density case. [OI] 63  $\mu m$  is the same within a factor of 2 in the high density case for all mechanical heating and CR rates, but does increase a factor 5 in the low density case. The critical density for excitation of the [OI] 63  $\mu m$  is  $n_{crit} = 5 \cdot 10^5 cm^{-3}$ , and the low density model is not even close to being thermalized, and temperature differences cause a large change in emitted flux. The [CII] 158  $\mu m$  has a very low critical density  $n_{crit} = 2.8 \cdot 10^3 cm^{-3}$ , and the increase in fluxes is not explained by the rise in temperature at small column densities. Additional flux is emitted in low density clouds, because there is no full transition to neutral carbon and CO, for the highest CR rates (see Section 2). This also explains why the two neutral carbon lines, [CI] 610  $\mu m$  and [CI] 370  $\mu m$ , show an increase in the high density models. The low density models have a maximum intensity at  $\zeta \sim 5 \cdot 10^{-15} s^{-1}$ , since for higher CR rates the main carbon budget remains in C<sup>+</sup>. The two ionized nitrogen lines, [NII] 205  $\mu m$  and [NII] 122  $\mu m$ , increase by 4 (3) orders of magnitude in the high (low) density case. Especially low density clouds are expected to yield detectable fluxes: the [NII] 122  $\mu m$  lines has only a 10 times weaker flux than the [CII] line at the highest CR rate. Unfortunately, O<sup>+</sup> does not have fine-structure transitions in the mid and far-infrared. Available transitions are in the visible and UV, and have very high excitation energies.

**H<sub>3</sub><sup>+</sup> 95  $\mu m$ :** This transition is calculated following the discussion in Pan & Oka (1986). The fluxes in the high density case



**Fig. 8.** Abundances of hydrogen and water chemistry for an XDR model with density  $n = 10^{5.5} cm^{-3}$  and  $F_x = 28.5 erg cm^{-2} s^{-1}$ .

are very similar to the [NII] 122  $\mu m$ , not extremely strong, but potentially detectable, when clouds are exposed to very large CR fluxes.

**HCN, HNC, and HCO<sup>+</sup>:** The HCN and HNC do not seem very helpful in the discussion of cosmic ray rates, as there are no obvious trends. The HCN/HNC ratio does show a response to mechanical heating as already pointed out in Loenen et al. (2008), and especially HCN is boosted by a few orders of magnitude. An exception is the high density with the high CR rate, where He<sup>+</sup> destroys the HCN and HNC very effectively. Also HCO<sup>+</sup> does not exhibit very obvious trends, except for very high mechanical heating rates (model set 1c).

**CO and <sup>13</sup>CO:** In the high density models, there is very little response when increasing the cosmic ray flux. Fluxes are boosted, when mechanical heating plays an important role in the energy budget of the gas, but, contrary to the HCN and HNC lines, it only affects high- $J$  transitions. When <sup>13</sup>CO line fluxes are also available, mechanical heating effects are potentially also seen in the lower- $J$  transitions ( $J \lesssim 3$ ). The CO to <sup>13</sup>CO line ratio increases, indicating smaller optical depths, while CO fluxes only decrease by a factor 2

#### 5. Key Diagnostics

The aim of this paper is to pinpoint potential line diagnostics that can be used to trace an enhanced cosmic ray radiation field and mechanical heating in the presence of starformation such as the central regions of Arp 220 and NGC 253. One of the remarkable results is that many commonly observed lines, such as, the [OI] 63  $\mu m$ , [CI] 609  $\mu m$ , the [CII] 158  $\mu m$  and the low- $J$  CO lines, show very moderate responses to high cosmic ray rates and mechanical feedback, when the medium is already exposed to a large amount of UV. This is a very useful result, since these lines can serve as a reference point to other lines fluxes, that are impacted.

**Table 6.** Line intensities for Model set 1a

Line	Cosmic ray rate (s <sup>-1</sup> )				
	5(-17)	5(-16)	5(-15)	5(-14)	5(-13)
Line intensities (erg s <sup>-1</sup> cm <sup>-2</sup> sr <sup>-1</sup> )					
[CII] 158 $\mu$ m	1.1(-3)	1.1(-3)	1.1(-3)	1.1(-3)	1.3(-3)
[CI] 610 $\mu$ m	3.7(-6)	3.9(-6)	4.2(-6)	4.8(-6)	1.1(-5)
[CI] 370 $\mu$ m	2.1(-5)	2.2(-5)	2.3(-5)	2.6(-5)	6.2(-5)
[OI] 63 $\mu$ m	7.8(-2)	7.8(-2)	7.8(-2)	8.2(-2)	9.2(-2)
[OI] 146 $\mu$ m	2.3(-3)	2.3(-3)	2.3(-3)	2.4(-3)	2.9(-3)
[NII] 205 $\mu$ m	4.4(-11)	4.4(-10)	4.7(-9)	5.5(-8)	4.2(-7)
[NII] 122 $\mu$ m	6.6(-10)	6.6(-9)	7.1(-8)	8.4(-7)	6.6(-6)
H <sub>3</sub> <sup>+</sup> 95 $\mu$ m	7.0(-10)	6.2(-9)	6.0(-8)	6.5(-7)	1.9(-6)
HCN $J = 1 - 0$	1.5(-8)	1.8(-8)	1.8(-8)	2.9(-8)	1.1(-8)
HCN $J = 2 - 1$	1.3(-7)	1.5(-7)	1.5(-7)	2.2(-7)	1.3(-7)
HCN $J = 3 - 2$	3.2(-7)	3.7(-7)	3.6(-7)	5.8(-7)	3.3(-7)
HCN $J = 4 - 3$	3.8(-7)	4.7(-7)	4.5(-7)	8.9(-7)	4.4(-7)
HCN $J = 5 - 4$	3.3(-7)	4.0(-7)	3.9(-7)	7.7(-7)	4.0(-7)
HCN $J = 6 - 5$	2.6(-7)	3.0(-7)	3.0(-7)	5.2(-7)	3.1(-7)
HCN $J = 7 - 6$	2.0(-7)	2.2(-7)	2.2(-7)	3.2(-7)	2.2(-7)
HNC $J = 1 - 0$	1.1(-8)	1.3(-8)	2.0(-8)	3.6(-8)	1.7(-8)
HNC $J = 2 - 1$	9.9(-8)	1.1(-7)	1.6(-7)	2.5(-7)	1.7(-7)
HNC $J = 3 - 2$	2.1(-7)	2.4(-7)	3.9(-7)	6.7(-7)	4.5(-7)
HNC $J = 4 - 3$	2.3(-7)	2.6(-7)	4.9(-7)	1.1(-6)	6.3(-7)
HNC $J = 5 - 4$	1.9(-7)	2.0(-7)	3.4(-7)	1.1(-6)	5.7(-7)
HNC $J = 6 - 5$	1.4(-7)	1.5(-7)	2.2(-7)	6.1(-7)	4.2(-7)
HNC $J = 7 - 6$	9.7(-8)	1.0(-7)	1.3(-7)	3.3(-7)	2.8(-7)
HCO <sup>+</sup> $J = 1 - 0$	2.7(-8)	1.0(-7)	1.5(-7)	1.6(-7)	5.5(-8)
HCO <sup>+</sup> $J = 2 - 1$	2.8(-7)	7.7(-7)	9.8(-7)	1.2(-6)	7.3(-7)
HCO <sup>+</sup> $J = 3 - 2$	8.1(-7)	2.2(-6)	2.7(-6)	3.3(-6)	3.1(-6)
HCO <sup>+</sup> $J = 4 - 3$	1.4(-6)	4.4(-6)	5.5(-6)	6.8(-6)	6.8(-6)
HCO <sup>+</sup> $J = 5 - 4$	1.6(-6)	7.2(-6)	9.4(-6)	1.2(-5)	9.4(-6)
HCO <sup>+</sup> $J = 6 - 5$	1.2(-6)	1.0(-5)	1.4(-5)	1.9(-5)	1.3(-5)
HCO <sup>+</sup> $J = 7 - 6$	8.2(-7)	1.2(-5)	2.0(-5)	2.8(-5)	1.5(-5)
CO $J = 1 - 0$	3.0(-7)	3.0(-7)	3.1(-7)	3.2(-7)	3.1(-7)
CO $J = 2 - 1$	2.9(-6)	3.0(-6)	3.0(-6)	3.3(-6)	3.9(-6)
CO $J = 3 - 2$	1.0(-5)	1.0(-5)	1.1(-5)	1.2(-5)	1.5(-5)
CO $J = 4 - 3$	2.4(-5)	2.4(-5)	2.5(-5)	2.8(-5)	3.9(-5)
CO $J = 5 - 4$	4.3(-5)	4.4(-5)	4.6(-5)	5.3(-5)	7.8(-5)
CO $J = 6 - 5$	6.7(-5)	6.8(-5)	7.1(-5)	8.4(-5)	1.3(-4)
CO $J = 7 - 6$	9.2(-5)	9.4(-5)	9.8(-5)	1.2(-4)	2.0(-4)
CO $J = 8 - 7$	1.1(-4)	1.1(-4)	1.2(-4)	1.5(-4)	2.8(-4)
CO $J = 9 - 8$	1.2(-4)	1.3(-4)	1.3(-4)	1.7(-4)	3.6(-4)
CO $J = 10 - 9$	1.1(-4)	1.2(-4)	1.2(-4)	1.8(-4)	4.3(-4)
CO $J = 11 - 10$	8.2(-5)	8.9(-5)	9.4(-5)	1.6(-4)	4.8(-4)
CO $J = 12 - 11$	3.8(-5)	4.3(-5)	4.8(-5)	1.1(-4)	5.0(-4)
CO $J = 13 - 12$	1.2(-5)	1.4(-5)	1.6(-5)	5.1(-5)	4.7(-4)
CO $J = 14 - 13$	4.7(-6)	5.2(-6)	5.7(-6)	1.8(-5)	3.8(-4)
CO $J = 17 - 16$	3.4(-6)	3.4(-6)	3.4(-6)	3.8(-6)	5.8(-5)
CO $J = 20 - 19$	3.6(-6)	3.6(-6)	3.6(-6)	3.5(-6)	7.8(-6)
CO $J = 24 - 23$	2.4(-6)	2.4(-6)	2.3(-6)	2.2(-6)	2.4(-6)
CO $J = 30 - 29$	4.9(-7)	4.9(-7)	4.8(-7)	4.4(-7)	4.9(-7)
CO $J = 35 - 34$	1.0(-7)	1.0(-7)	1.0(-7)	9.9(-8)	1.3(-7)
<sup>13</sup> CO $J = 1 - 0$	4.1(-8)	4.1(-8)	4.0(-8)	3.6(-8)	1.4(-8)
<sup>13</sup> CO $J = 2 - 1$	7.9(-7)	7.9(-7)	7.9(-7)	7.6(-7)	3.7(-7)
<sup>13</sup> CO $J = 3 - 2$	3.4(-6)	3.4(-6)	3.4(-6)	3.5(-6)	2.2(-6)
<sup>13</sup> CO $J = 4 - 3$	8.4(-6)	8.5(-6)	8.5(-6)	9.1(-6)	7.0(-6)
<sup>13</sup> CO $J = 5 - 4$	1.5(-5)	1.5(-5)	1.5(-5)	1.7(-5)	1.5(-5)
<sup>13</sup> CO $J = 6 - 5$	2.2(-5)	2.2(-5)	2.2(-5)	2.6(-5)	2.7(-5)
<sup>13</sup> CO $J = 7 - 6$	2.5(-5)	2.6(-5)	2.6(-5)	3.3(-5)	3.9(-5)
<sup>13</sup> CO $J = 8 - 7$	2.3(-5)	2.4(-5)	2.5(-5)	3.4(-5)	5.0(-5)
<sup>13</sup> CO $J = 9 - 8$	1.6(-5)	1.7(-5)	1.8(-5)	2.8(-5)	5.6(-5)
<sup>13</sup> CO $J = 10 - 9$	8.3(-6)	9.1(-6)	9.7(-6)	1.8(-5)	5.5(-5)
<sup>13</sup> CO $J = 11 - 10$	3.4(-6)	3.8(-6)	4.2(-6)	9.6(-6)	4.7(-5)
<sup>13</sup> CO $J = 12 - 11$	1.2(-6)	1.4(-6)	1.5(-6)	4.2(-6)	3.6(-5)
<sup>13</sup> CO $J = 13 - 12$	4.0(-7)	4.4(-7)	5.0(-7)	1.6(-6)	2.4(-5)
<sup>13</sup> CO $J = 14 - 13$	1.5(-7)	1.6(-7)	1.8(-7)	5.7(-7)	1.4(-5)

**Table 7.** Line intensities for Model set 1b

Line	Cosmic ray rate (s <sup>-1</sup> )				
	5(-17)	5(-16)	5(-15)	5(-14)	5(-13)
Line intensities (erg s <sup>-1</sup> cm <sup>-2</sup> sr <sup>-1</sup> )					
[CII] 158 $\mu$ m	1.1(-3)	1.1(-3)	1.1(-3)	1.2(-3)	1.3(-3)
[CI] 610 $\mu$ m	3.4(-6)	3.6(-6)	3.9(-6)	4.9(-6)	7.3(-6)
[CI] 370 $\mu$ m	2.4(-5)	2.5(-5)	2.8(-5)	3.4(-5)	5.2(-5)
[OI] 63 $\mu$ m	9.3(-2)	9.4(-2)	9.4(-2)	9.8(-2)	1.1(-1)
[OI] 146 $\mu$ m	3.7(-3)	3.7(-3)	3.8(-3)	3.9(-3)	4.1(-3)
[NII] 205 $\mu$ m	4.7(-11)	4.7(-10)	5.0(-9)	5.7(-8)	4.3(-7)
[NII] 122 $\mu$ m	7.2(-10)	7.2(-9)	7.7(-8)	8.8(-7)	6.7(-6)
H <sub>3</sub> <sup>+</sup> 95 $\mu$ m	3.6(-9)	3.8(-8)	3.6(-7)	2.8(-6)	6.0(-6)
HCN $J = 1 - 0$	3.1(-8)	5.8(-8)	1.2(-7)	1.3(-7)	2.0(-8)
HCN $J = 2 - 1$	2.9(-7)	4.3(-7)	6.7(-7)	7.4(-7)	2.8(-7)
HCN $J = 3 - 2$	8.3(-7)	1.2(-6)	1.9(-6)	2.0(-6)	8.1(-7)
HCN $J = 4 - 3$	1.6(-6)	2.6(-6)	4.1(-6)	4.4(-6)	1.5(-6)
HCN $J = 5 - 4$	2.0(-6)	4.2(-6)	7.4(-6)	8.1(-6)	2.0(-6)
HCN $J = 6 - 5$	1.8(-6)	5.2(-6)	1.2(-5)	1.3(-5)	1.9(-6)
HCN $J = 7 - 6$	1.5(-6)	4.6(-6)	1.5(-5)	1.8(-5)	1.6(-6)
HNC $J = 1 - 0$	2.2(-8)	3.0(-8)	5.5(-8)	6.0(-8)	2.2(-8)
HNC $J = 2 - 1$	2.3(-7)	2.9(-7)	4.3(-7)	4.7(-7)	2.8(-7)
HNC $J = 3 - 2$	6.5(-7)	8.2(-7)	1.2(-6)	1.3(-6)	8.1(-7)
HNC $J = 4 - 3$	1.1(-6)	1.5(-6)	2.5(-6)	2.8(-6)	1.5(-6)
HNC $J = 5 - 4$	1.2(-6)	2.0(-6)	4.0(-6)	4.5(-6)	1.9(-6)
HNC $J = 6 - 5$	1.1(-6)	1.8(-6)	4.7(-6)	5.6(-6)	1.8(-6)
HNC $J = 7 - 6$	9.2(-7)	1.5(-6)	3.8(-6)	4.9(-6)	1.5(-6)
HCO <sup>+</sup> $J = 1 - 0$	1.9(-8)	1.4(-7)	3.3(-7)	5.5(-7)	1.9(-7)
HCO <sup>+</sup> $J = 2 - 1$	3.8(-7)	1.7(-6)	2.9(-6)	3.9(-6)	2.5(-6)
HCO <sup>+</sup> $J = 3 - 2$	1.3(-6)	4.7(-6)	6.5(-6)	8.2(-6)	6.6(-6)
HCO <sup>+</sup> $J = 4 - 3$	2.7(-6)	9.5(-6)	1.3(-5)	1.5(-5)	1.3(-5)
HCO <sup>+</sup> $J = 5 - 4$	4.1(-6)	1.7(-5)	2.3(-5)	2.7(-5)	2.3(-5)
HCO <sup>+</sup> $J = 6 - 5$	4.9(-6)	2.7(-5)	3.8(-5)	4.5(-5)	3.7(-5)
HCO <sup>+</sup> $J = 7 - 6$	4.5(-6)	3.9(-5)	5.9(-5)	7.1(-5)	5.5(-5)
CO $J = 1 - 0$	4.2(-7)	4.1(-7)	4.1(-7)	4.0(-7)	3.6(-7)
CO $J = 2 - 1$	6.1(-6)	6.1(-6)	6.2(-6)	6.1(-6)	5.8(-6)
CO $J = 3 - 2$	2.5(-5)	2.5(-5)	2.5(-5)	2.5(-5)	2.4(-5)
CO $J = 4 - 3$	6.3(-5)	6.3(-5)	6.4(-5)	6.4(-5)	6.4(-5)
CO $J = 5 - 4$	1.3(-4)	1.3(-4)	1.3(-4)	1.3(-4)	1.3(-4)
CO $J = 6 - 5$	2.2(-4)	2.2(-4)	2.3(-4)	2.3(-4)	2.3(-4)
CO $J = 7 - 6$	3.5(-4)	3.6(-4)	3.6(-4)	3.6(-4)	3.7(-4)
CO $J = 8 - 7$	5.2(-4)	5.2(-4)	5.3(-4)	5.3(-4)	5.5(-4)
CO $J = 9 - 8$	7.1(-4)	7.3(-4)	7.3(-4)	7.3(-4)	7.7(-4)
CO $J = 10 - 9$	9.4(-4)	9.6(-4)	9.7(-4)	9.7(-4)	1.0(-3)
CO $J = 11 - 10$	1.2(-3)	1.2(-3)	1.2(-3)	1.2(-3)	1.3(-3)
CO $J = 12 - 11$	1.5(-3)	1.5(-3)	1.5(-3)	1.5(-3)	1.6(-3)
CO $J = 13 - 12$	1.7(-3)	1.8(-3)	1.8(-3)	1.7(-3)	1.8(-3)
CO $J = 14 - 13$	2.0(-3)	2.0(-3)	2.0(-3)	2.0(-3)	2.1(-3)
CO $J = 17 - 16$	2.2(-3)	2.4(-3)	2.3(-3)	2.2(-3)	2.3(-3)
CO $J = 20 - 19$	9.1(-4)	1.1(-3)	1.0(-3)	8.7(-4)	1.2(-3)
CO $J = 24 - 23$	2.7(-5)	3.7(-5)	3.1(-5)	2.6(-5)	5.5(-5)
CO $J = 30 - 29$	8.0(-7)	8.1(-7)	7.8(-7)	7.2(-7)	7.8(-7)
CO $J = 35 - 34$	1.7(-7)	1.7(-7)	1.7(-7)	1.6(-7)	1.9(-7)
<sup>13</sup> CO $J = 1 - 0$	1.5(-8)	1.4(-8)	1.4(-8)	1.4(-8)	1.1(-8)
<sup>13</sup> CO $J = 2 - 1$	4.3(-7)	4.2(-7)	4.2(-7)	4.0(-7)	3.2(-7)
<sup>13</sup> CO $J = 3 - 2$	2.9(-6)	2.8(-6)	2.8(-6)	2.7(-6)	2.2(-6)
<sup>13</sup> CO $J = 4 - 3$	1.0(-5)	1.0(-5)	1.0(-5)	9.6(-6)	7.9(-6)
<sup>13</sup> CO $J = 5 - 4$	2.6(-5)	2.5(-5)	2.5(-5)	2.4(-5)	2.0(-5)
<sup>13</sup> CO $J = 6 - 5$	5.1(-5)	5.0(-5)	5.0(-5)	4.8(-5)	4.1(-5)
<sup>13</sup> CO $J = 7 - 6$	8.5(-5)	8.5(-5)	8.5(-5)	8.1(-5)	7.0(-5)
<sup>13</sup> CO $J = 8 - 7$	1.3(-4)	1.3(-4)	1.3(-4)	1.2(-4)	1.1(-4)
<sup>13</sup> CO $J = 9 - 8$	1.7(-4)	1.7(-4)	1.7(-4)	1.7(-4)	1.5(-4)
<sup>13</sup> CO $J = 10 - 9$	2.1(-4)	2.1(-4)	2.1(-4)	2.0(-4)	1.9(-4)
<sup>13</sup> CO $J = 11 - 10$	2.4(-4)	2.5(-4)	2.4(-4)	2.3(-4)	2.2(-4)
<sup>13</sup> CO $J = 12 - 11$	2.5(-4)	2.6(-4)	2.5(-4)	2.4(-4)	2.3(-4)
<sup>13</sup> CO $J = 13 - 12$	2.4(-4)	2.5(-4)	2.4(-4)	2.3(-4)	2.4(-4)
<sup>13</sup> CO $J = 14 - 13$	2.0(-4)	2.2(-4)	2.1(-4)	2.0(-4)	2.2(-4)

**Table 8.** Line intensities for Model set 1c

Line	Cosmic ray rate ( $\text{s}^{-1}$ )				
	5(-17)	5(-16)	5(-15)	5(-14)	5(-13)
Line intensities ( $\text{erg s}^{-1} \text{cm}^{-2} \text{sr}^{-1}$ )					
[CII] 158 $\mu\text{m}$	1.1(-3)	1.1(-3)	1.1(-3)	1.1(-3)	1.3(-3)
[CI] 610 $\mu\text{m}$	8.3(-7)	1.3(-6)	2.5(-6)	3.8(-6)	7.7(-6)
[CI] 370 $\mu\text{m}$	7.1(-6)	1.1(-5)	2.1(-5)	3.2(-5)	6.3(-5)
[OI] 63 $\mu\text{m}$	1.1(-1)	1.1(-1)	1.1(-1)	1.3(-1)	1.5(-1)
[OI] 146 $\mu\text{m}$	3.9(-3)	3.9(-3)	4.1(-3)	5.4(-3)	6.7(-3)
[NII] 205 $\mu\text{m}$	7.3(-11)	7.3(-10)	7.5(-9)	7.1(-8)	4.7(-7)
[NII] 122 $\mu\text{m}$	1.1(-9)	1.1(-8)	1.1(-7)	1.1(-6)	7.4(-6)
$\text{H}_3^+$ 95 $\mu\text{m}$	1.8(-9)	1.7(-8)	1.8(-7)	2.1(-6)	9.9(-6)
HCN $J = 1 - 0$	3.9(-5)	4.0(-5)	2.2(-5)	4.7(-6)	1.8(-7)
HCN $J = 2 - 1$	2.1(-5)	2.0(-5)	1.7(-5)	9.5(-6)	2.7(-6)
HCN $J = 3 - 2$	1.8(-5)	1.9(-5)	1.8(-5)	1.4(-5)	4.1(-6)
HCN $J = 4 - 3$	3.0(-5)	3.1(-5)	3.0(-5)	2.6(-5)	1.2(-5)
HCN $J = 5 - 4$	5.2(-5)	5.3(-5)	5.3(-5)	4.4(-5)	2.0(-5)
HCN $J = 6 - 5$	9.1(-5)	9.3(-5)	9.3(-5)	7.5(-5)	3.5(-5)
HCN $J = 7 - 6$	1.5(-4)	1.6(-4)	1.6(-4)	1.2(-4)	5.4(-5)
HNC $J = 1 - 0$	7.9(-7)	6.0(-7)	4.4(-7)	1.2(-7)	1.7(-8)
HNC $J = 2 - 1$	3.3(-6)	2.9(-6)	2.4(-6)	1.1(-6)	3.0(-7)
HNC $J = 3 - 2$	6.4(-6)	5.9(-6)	5.2(-6)	4.4(-6)	1.0(-6)
HNC $J = 4 - 3$	1.3(-5)	1.2(-5)	1.1(-5)	7.4(-6)	2.1(-6)
HNC $J = 5 - 4$	2.4(-5)	2.2(-5)	2.0(-5)	1.3(-5)	3.1(-6)
HNC $J = 6 - 5$	4.1(-5)	3.8(-5)	3.4(-5)	2.0(-5)	3.4(-6)
HNC $J = 7 - 6$	6.8(-5)	6.2(-5)	5.5(-5)	3.0(-5)	3.3(-6)
$\text{HCO}^+ J = 1 - 0$	4.9(-9)	1.0(-8)	3.9(-8)	1.9(-7)	4.9(-7)
$\text{HCO}^+ J = 2 - 1$	1.4(-7)	2.7(-7)	8.8(-7)	3.1(-6)	7.6(-6)
$\text{HCO}^+ J = 3 - 2$	6.6(-7)	1.2(-6)	3.2(-6)	8.7(-6)	1.7(-5)
$\text{HCO}^+ J = 4 - 3$	1.7(-6)	2.7(-6)	6.8(-6)	1.7(-5)	3.1(-5)
$\text{HCO}^+ J = 5 - 4$	2.7(-6)	4.2(-6)	1.2(-5)	3.0(-5)	5.0(-5)
$\text{HCO}^+ J = 6 - 5$	3.2(-6)	5.1(-6)	1.7(-5)	4.7(-5)	7.9(-5)
$\text{HCO}^+ J = 7 - 6$	3.3(-6)	5.2(-6)	2.2(-5)	7.0(-5)	1.2(-4)
CO $J = 1 - 0$	2.1(-7)	2.3(-7)	2.7(-7)	2.9(-7)	2.3(-7)
CO $J = 2 - 1$	5.5(-6)	5.9(-6)	6.7(-6)	6.9(-6)	5.7(-6)
CO $J = 3 - 2$	3.1(-5)	3.3(-5)	3.6(-5)	3.7(-5)	3.2(-5)
CO $J = 4 - 3$	9.6(-5)	1.0(-4)	1.1(-4)	1.1(-4)	9.8(-5)
CO $J = 5 - 4$	2.2(-4)	2.2(-4)	2.4(-4)	2.4(-4)	2.2(-4)
CO $J = 6 - 5$	4.1(-4)	4.2(-4)	4.4(-4)	4.5(-4)	4.2(-4)
CO $J = 7 - 6$	6.8(-4)	7.0(-4)	7.3(-4)	7.5(-4)	7.0(-4)
CO $J = 8 - 7$	1.0(-3)	1.1(-3)	1.1(-3)	1.2(-3)	1.1(-3)
CO $J = 9 - 8$	1.5(-3)	1.5(-3)	1.6(-3)	1.6(-3)	1.6(-3)
CO $J = 10 - 9$	2.0(-3)	2.1(-3)	2.2(-3)	2.2(-3)	2.1(-3)
CO $J = 11 - 10$	2.6(-3)	2.7(-3)	2.9(-3)	2.9(-3)	2.8(-3)
CO $J = 12 - 11$	3.3(-3)	3.4(-3)	3.6(-3)	3.7(-3)	3.6(-3)
CO $J = 13 - 12$	4.0(-3)	4.1(-3)	4.4(-3)	4.5(-3)	4.5(-3)
CO $J = 14 - 13$	4.7(-3)	4.9(-3)	5.2(-3)	5.4(-3)	5.4(-3)
CO $J = 17 - 16$	6.5(-3)	6.8(-3)	7.3(-3)	7.6(-3)	8.1(-3)
CO $J = 20 - 19$	6.6(-3)	7.0(-3)	7.7(-3)	8.3(-3)	9.6(-3)
CO $J = 24 - 23$	1.8(-3)	2.1(-3)	2.9(-3)	3.7(-3)	6.3(-3)
CO $J = 30 - 29$	3.7(-5)	4.2(-5)	5.4(-5)	6.9(-5)	2.1(-4)
CO $J = 35 - 34$	3.1(-6)	3.2(-6)	3.5(-6)	3.6(-6)	7.6(-6)
$^{13}\text{CO } J = 1 - 0$	5.5(-9)	6.1(-9)	7.2(-9)	7.6(-9)	5.6(-9)
$^{13}\text{CO } J = 2 - 1$	1.7(-7)	1.9(-8)	2.3(-7)	2.4(-7)	1.7(-7)
$^{13}\text{CO } J = 3 - 2$	1.2(-6)	1.4(-6)	1.6(-6)	1.7(-6)	1.3(-6)
$^{13}\text{CO } J = 4 - 3$	5.0(-6)	5.5(-6)	6.5(-6)	6.8(-6)	5.0(-6)
$^{13}\text{CO } J = 5 - 4$	1.4(-5)	1.5(-5)	1.8(-5)	1.9(-5)	1.4(-5)
$^{13}\text{CO } J = 6 - 5$	3.2(-5)	3.5(-5)	4.1(-5)	4.3(-5)	3.2(-5)
$^{13}\text{CO } J = 7 - 6$	6.1(-5)	6.6(-5)	7.8(-5)	8.2(-5)	6.3(-5)
$^{13}\text{CO } J = 8 - 7$	1.0(-4)	1.1(-4)	1.3(-4)	1.4(-4)	1.1(-4)
$^{13}\text{CO } J = 9 - 8$	1.6(-4)	1.7(-4)	2.0(-4)	2.1(-4)	1.7(-4)
$^{13}\text{CO } J = 10 - 9$	2.2(-4)	2.4(-4)	2.8(-4)	3.0(-4)	2.4(-4)
$^{13}\text{CO } J = 11 - 10$	2.9(-4)	3.1(-4)	3.6(-4)	3.9(-4)	3.3(-4)
$^{13}\text{CO } J = 12 - 11$	3.5(-4)	3.8(-4)	4.4(-4)	4.8(-4)	4.2(-4)
$^{13}\text{CO } J = 13 - 12$	4.0(-4)	4.3(-4)	5.1(-4)	5.5(-4)	5.1(-4)
$^{13}\text{CO } J = 14 - 13$	4.2(-4)	4.6(-4)	5.4(-4)	6.0(-4)	5.9(-4)

**Table 9.** Line intensities for Model set 2

Line	Cosmic ray rate ( $\text{s}^{-1}$ )				
	5(-17)	5(-16)	5(-15)	5(-14)	5(-13)
Line intensities ( $\text{erg s}^{-1} \text{cm}^{-2} \text{sr}^{-1}$ )					
[CII] 158 $\mu\text{m}$	4.4(-4)	4.7(-4)	5.8(-4)	8.6(-4)	1.2(-3)
[CI] 610 $\mu\text{m}$	3.6(-6)	4.6(-6)	9.7(-6)	6.6(-6)	2.8(-6)
[CI] 370 $\mu\text{m}$	1.0(-5)	1.3(-5)	3.5(-5)	3.0(-5)	1.5(-5)
[OI] 63 $\mu\text{m}$	4.5(-4)	6.4(-4)	1.3(-3)	2.4(-3)	2.9(-3)
[OI] 146 $\mu\text{m}$	5.5(-6)	7.0(-6)	1.1(-5)	2.1(-5)	3.1(-5)
[NII] 205 $\mu\text{m}$	6.6(-9)	5.3(-8)	3.7(-7)	2.1(-6)	7.6(-6)
[NII] 122 $\mu\text{m}$	4.2(-7)	7.2(-7)	5.5(-6)	3.3(-5)	1.1(-4)
$\text{H}_3^+$ 95 $\mu\text{m}$	4.7(-10)	7.0(-9)	3.2(-8)	2.0(-8)	3.6(-9)
CO $J = 1 - 0$	7.6(-8)	1.3(-7)	5.0(-8)	2.8(-9)	5.2(-12)
CO $J = 2 - 1$	4.0(-7)	6.5(-7)	4.4(-7)	5.3(-8)	1.2(-10)
CO $J = 3 - 2$	1.5(-6)	2.0(-6)	1.1(-6)	1.4(-7)	3.6(-10)
CO $J = 4 - 3$	4.7(-6)	5.7(-6)	1.4(-6)	1.4(-7)	4.2(-10)
CO $J = 5 - 4$	1.2(-5)	1.4(-5)	7.6(-7)	8.9(-8)	2.9(-10)
CO $J = 6 - 5$	2.2(-5)	2.6(-5)	2.7(-7)	4.1(-8)	1.6(-10)
CO $J = 7 - 6$	3.2(-5)	4.1(-5)	7.5(-8)	1.6(-8)	7.0(-11)
CO $J = 8 - 7$	3.4(-5)	5.3(-5)	1.9(-8)	5.3(-9)	2.8(-11)
CO $J = 9 - 8$	2.3(-5)	5.1(-5)	4.4(-9)	1.6(-9)	1.1(-11)
CO $J = 10 - 9$	2.9(-6)	2.7(-5)	1.1(-9)	4.9(-10)	4.3(-12)
CO $J = 11 - 10$	7.2(-9)	1.8(-6)	3.4(-10)	1.5(-10)	2.0(-12)
CO $J = 12 - 11$	5.0(-12)	4.0(-9)	1.1(-10)	5.2(-11)	1.1(-12)
CO $J = 13 - 12$	3.6(-13)	4.3(-11)	4.0(-11)	1.9(-11)	6.5(-13)
CO $J = 14 - 13$	1.0(-13)	2.1(-12)	1.2(-11)	5.8(-12)	1.8(-13)
$^{13}\text{CO } J = 1 - 0$	3.1(-8)	4.6(-8)	1.6(-9)	5.1(-11)	9.1(-14)
$^{13}\text{CO } J = 2 - 1$	1.6(-7)	2.6(-7)	2.5(-8)	1.2(-9)	2.4(-12)
$^{13}\text{CO } J = 3 - 2$	3.3(-7)	6.4(-7)	5.3(-8)	3.9(-9)	9.5(-12)
$^{13}\text{CO } J = 4 - 3$	2.0(-7)	7.9(-7)	4.6(-8)	5.0(-9)	1.4(-11)
$^{13}\text{CO } J = 5 - 4$	2.0(-8)	2.5(-7)	2.6(-8)	3.9(-9)	1.2(-11)
$^{13}\text{CO } J = 6 - 5$	1.9(-9)	4.4(-8)	1.1(-8)	2.3(-9)	8.2(-12)
$^{13}\text{CO } J = 7 - 6$	1.2(-10)	7.5(-9)	4.4(-9)	1.2(-9)	4.7(-12)
$^{13}\text{CO } J = 8 - 7$	9.8(-12)	1.1(-9)	1.5(-9)	5.2(-10)	2.4(-12)

### 5.1. Tracers of Mechanical Heating

Mechanical heating is only increasing the temperature of the gas, leaving the ionization fraction unaffected. Tracing this heating mechanism with molecules that contain activation barriers in their formation route is thus very useful. Lines of, e.g., HCN and  $\text{H}_2\text{O}$  are enhanced with respect to the aforementioned fine-structure lines, especially for the highest considered mechanical heating rate. It was already pointed out by Loenen et al. (2008) that the HCN/HNC line ratios increase when mechanical heating is important, since at high temperatures the HNC will be driven in to HCN (see also Section 2). Moreover, the HCN/CO line ratios also increase when mechanical heating effects are important, but the interpretation of an observed ratio is not straightforward, because the lines trace slightly different regions.

### 5.2. Tracers of Enhanced Cosmic Ray Rates

The [NII] fine-structure lines show a very strong response to enhanced cosmic ray rates, independent of mechanical heating effects. The main concern with these lines, however, is that one has to disentangle the contributions arising from these CR exposed clouds and HII regions, that also contribute a significant amount of [NII] emission in starforming environments.

Most promising would be the study of lines from species important in the water chemistry, especially when the ionized water related species are considered. The OH to  $\text{H}_2\text{O}$  column density ratio varies over two to three orders of magnitude for the cosmic ray rates considered, from  $\sim 5 \cdot 10^{-3}$  ( $\zeta = 5.0 \cdot 10^{-17} \text{ s}^{-1}$ ) to  $\sim 1 - 3$  ( $\zeta = 5.0 \cdot 10^{-13} \text{ s}^{-1}$ ) in the high density case, and

$\sim 0.2$  to  $\sim 400$  in the low density case. So generally the OH lines are expected to be stronger in comparison to the water lines for higher cosmic ray rates. Fig. 8 shows an XDR model with density  $n = 10^{5.5} \text{ cm}^{-3}$ , and radiation field  $F_X = 28.5 \text{ erg cm}^{-2} \text{ s}^{-1}$  (a radiation field at  $\sim 170$  pc distance from a typical AGN with  $L_X = 10^{44} \text{ erg/s}$ ). From this we derive that the ratio varies between  $\sim 8$  (integrated up to  $N_H = 3 \cdot 10^{22} \text{ cm}^{-2}$ ) and  $\sim 1$  ( $N_H = 10^{24} \text{ cm}^{-2}$ ). So for very high CR rates, the ratios become comparable to a typical X-ray illuminated cloud.

Van der Tak et al. (2008) already pointed out that the  $\text{H}_3\text{O}^+/\text{H}_2\text{O}$  ratio is affected by either cosmic rays or X-rays. The high density models show variations over 1 to 2 orders of magnitude in the high density case. Unfortunately, the interpretation is not entirely unambiguous, since the  $\text{H}_3\text{O}^+$  abundance decreases for the highest CR rates. Also, clouds illuminated by high CR rates have similar ratios as those exposed to X-rays, namely  $(1 - 6) \cdot 10^{-3}$  ( $\zeta = 5 \cdot 10^{-14} \text{ s}^{-1}$ ) and  $(5 - 10) \cdot 10^{-3}$  ( $\zeta = 5 \cdot 10^{-13} \text{ s}^{-1}$ ) for models set 1, and between  $15 - 4 \cdot 10^{-3}$  (depending on the size of the cloud) for the XDR model shown in Fig. 8.

The current study reveals that additional observations of  $\text{OH}^+$  and  $\text{H}_2\text{O}^+$  might help out in distinguishing very high CR rates from a typical XDR. The  $\text{OH}^+$  and  $\text{H}_2\text{O}^+$  are significantly enhanced for CR rates that are  $10^3 - 10^4$  times larger than the accepted Milky Way value, but not as much as in the XDR.  $\text{OH}^+/\text{OH}$  and  $\text{H}_2\text{O}^+/\text{H}_2\text{O}$  column density ratios can be as high as  $(3 - 5) \cdot 10^{-4}$  to  $(2 - 14) \cdot 10^{-4}$ , respectively, compared to  $(250 - 7.5) \cdot 10^{-4}$  and  $(64 - 4) \cdot 10^{-3}$  ( $N_H = 3 \cdot 10^{22} - 10^{24} \text{ cm}^{-2}$ ). XDRs and regions with enhanced CR rates can be distinguished when all species are considered.

In this paper, no attempt is made to model lines from these species. As already pointed out in, e.g., González-Alfonso et al. (2008), the radiation transfer of OH and  $\text{H}_2\text{O}$  involves the consideration of both collisions and radiation pumping, which is beyond the scope of this paper. Also,  $\text{OH}^+$  and  $\text{H}_2\text{O}^+$  lines are not easily modeled. These species have formation and destruction times scales that are similar those for excitation. Besides that, collisional cross sections are unavailable at the moment, and quantum mechanical calculations are needed to obtain them.

## 6. Outlook

$\text{OH}^+$  and  $\text{H}_2\text{O}^+$  have already been detected in a number of sources:

- van der Werf et al. (2010) show  $\text{OH}^+$  and  $\text{H}_2\text{O}^+$  emission lines in the ULIRG Mrk231, which are about 30 percent of strength of the CO(5-6) to CO(13-12) lines. The paper show that these lines are the result from AGN activity in Mrk231.
- In the Milky Way,  $\text{OH}^+$  has been detected in absorption toward Sagittarius B2 using the Atacama Pathfinder Experiment (APEX) by Wyrowski et al. (2010), finding a column density of  $2.4 \cdot 10^{15} \text{ cm}^{-2}$ . Ossenkopf et al. (2010) found  $\text{H}_2\text{O}^+$  in absorption toward, NGC 6334, DR21, again Sgr B2, obtaining column densities of  $7.2 \cdot 10^{12} \text{ cm}^{-2}$ ,  $2.3 \cdot 10^{13} \text{ cm}^{-2}$ , and  $1.1 \cdot 10^{15} \text{ cm}^{-2}$ , respectively. These galactic observations relate these species to the diffuse ISM.

Extensive modeling of the excitation of water related species is very timely, since more and more observations will be available in a very short timeframe from observations with the recently launched *Herschel* Space Telescope.

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